

New Journal of Chemistry

Supplementary Information

Mn(III)-Mediated Cascade Cyclization of 1-(Azidomethyl)-2-Isocyanoarenes with Organoboronic acids: Construction of Quinazoline Derivatives

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1. Crystal structural data for compound 3a (CCDC 1911305)

Bond precision: C-C = 0.0039 Å Wavelength: 0.71073

Cell: a= 18.604 (5) b= 5.0525 (12) c= 11.244 (3)

alpha= 90 beta= 90 gamma= 90 Temperature: 296K

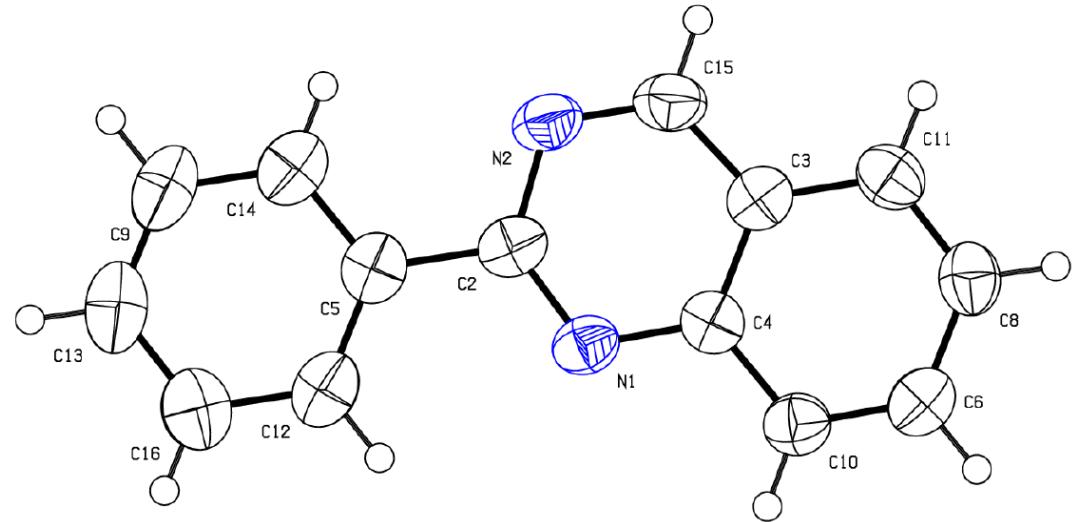
	Calculated
Volume	1056.9 (5)
Space group	P c a 21
Hall group	P 2c -2ac
Moiety formula	C14 H10 N2
Sum formula	C14 H10 N2
Mr	206.24
Dx, g cm ⁻³	1.296
Z	4
Mu (mm ⁻¹)	0.078
F000	432.0
F000'	432.14
h, k, lmax	24, 6, 14
Nref	2417 [1272]

Data completeness= 0.997 Theta (max)= 27.482

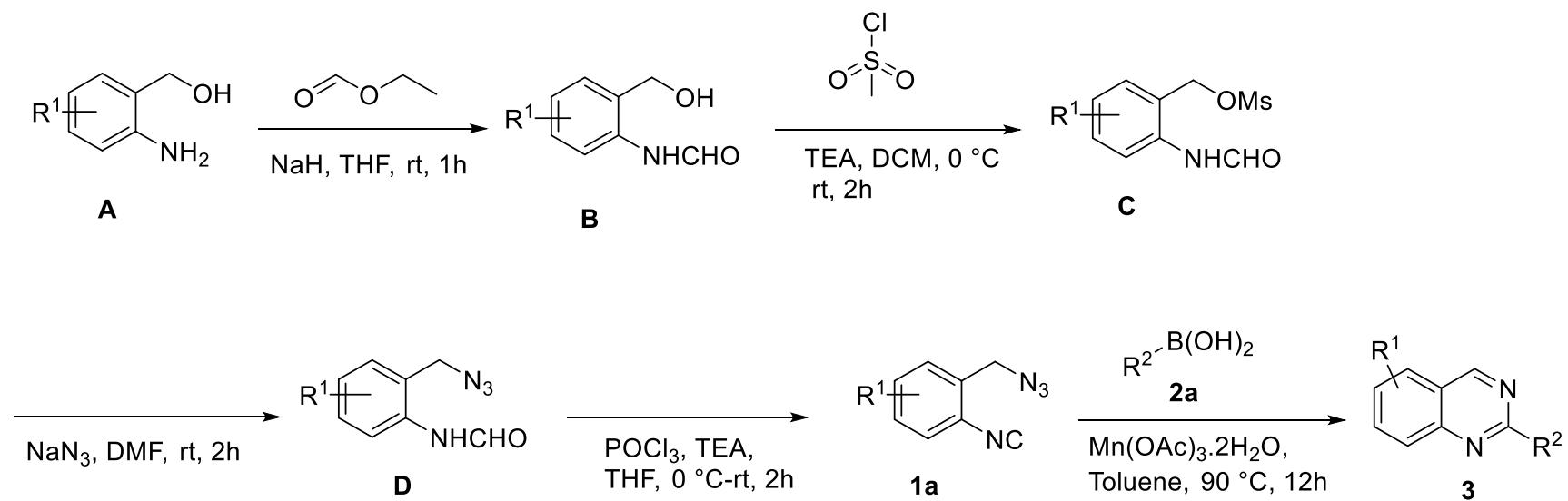
R (reflections) = 0.0597 (1575) wR2 (reflections) = 0.1449 (2374)

S = 1.070 Npar = 154

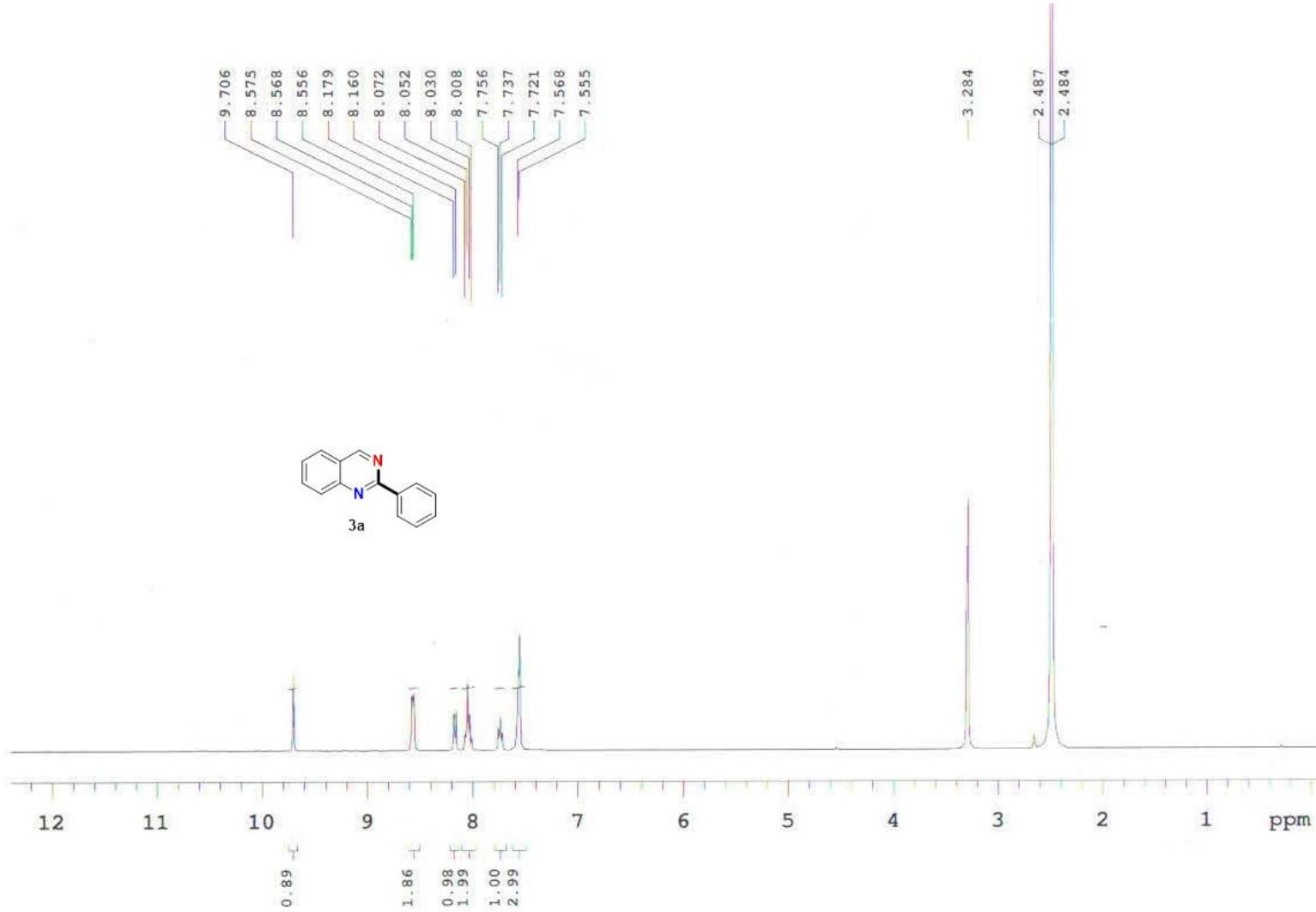
ORTEP diagram for compound 3a (50% ellipsoid probability)

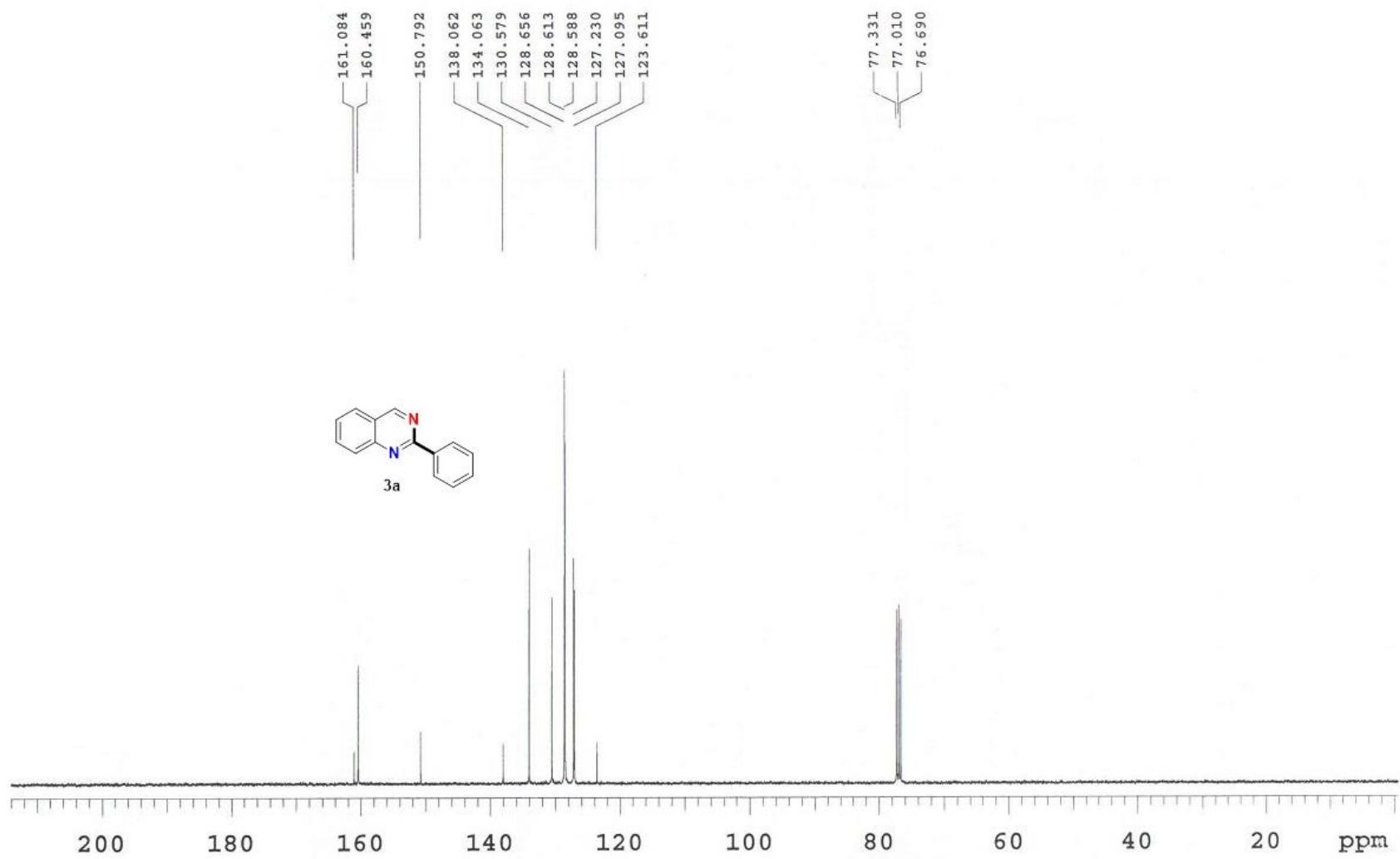


2. Reaction Schemes for Preparation of Substrates and Products

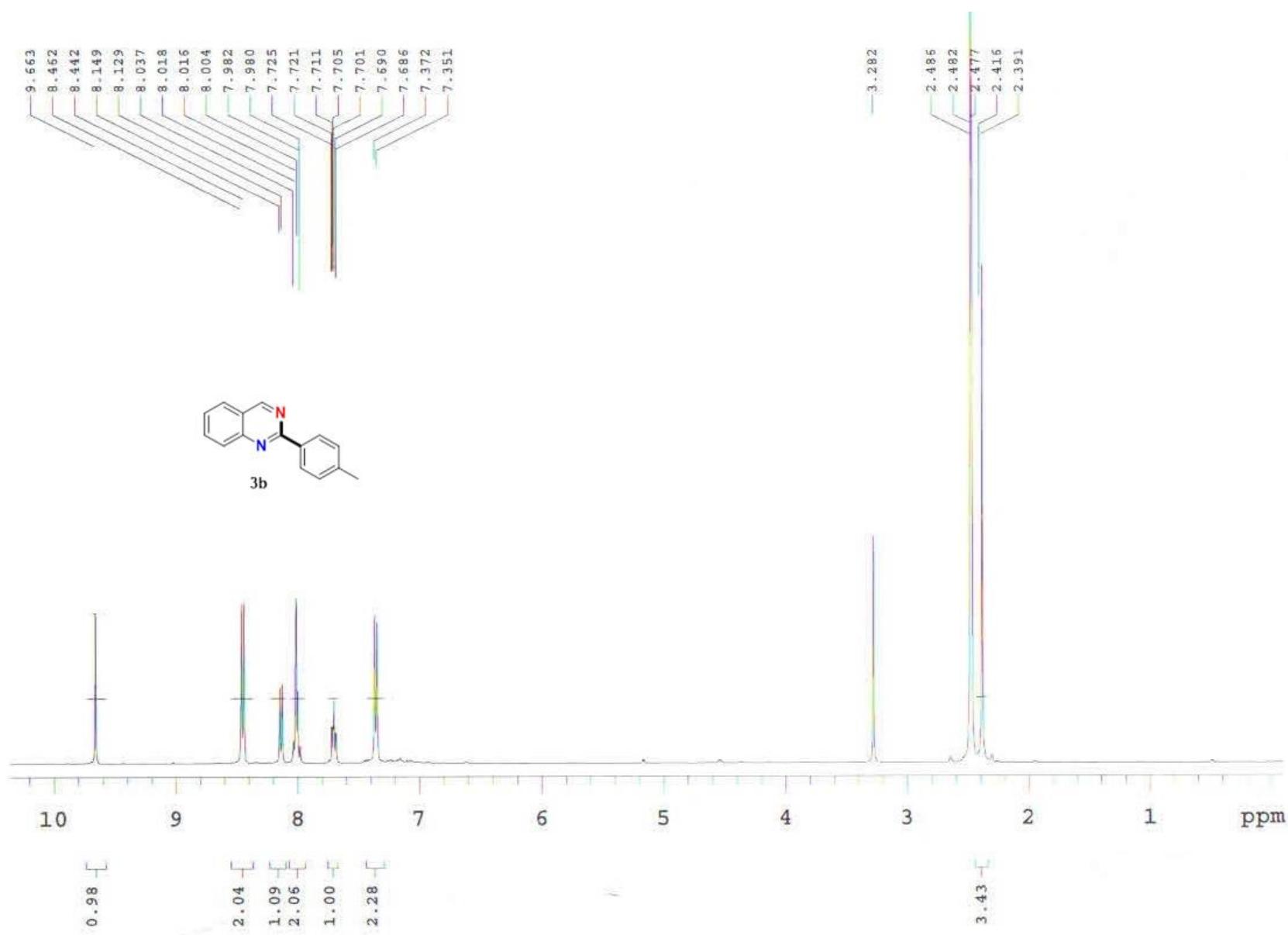


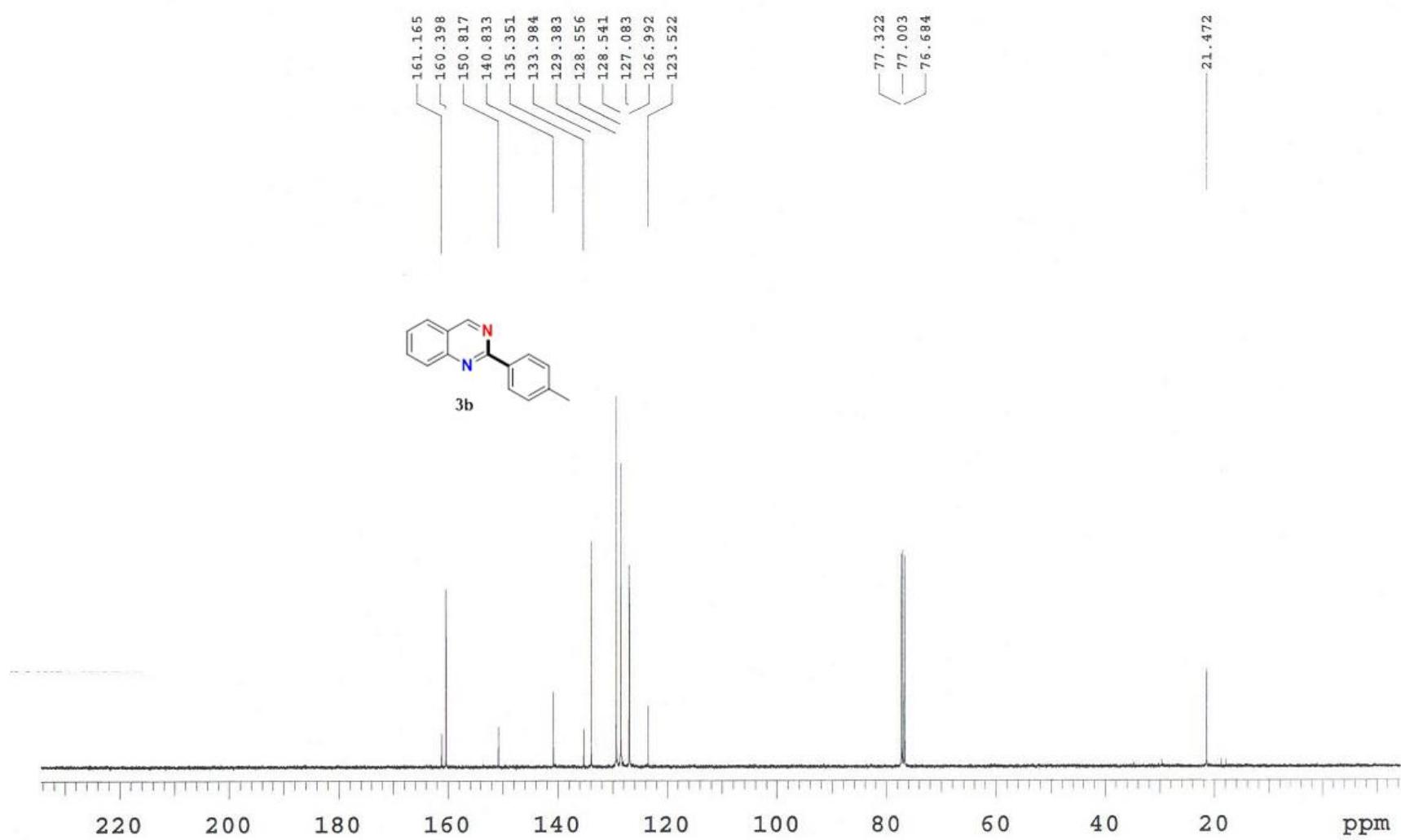
3. Copies of ^1H , ^{13}C NMR and ^{19}F NMR for Final products

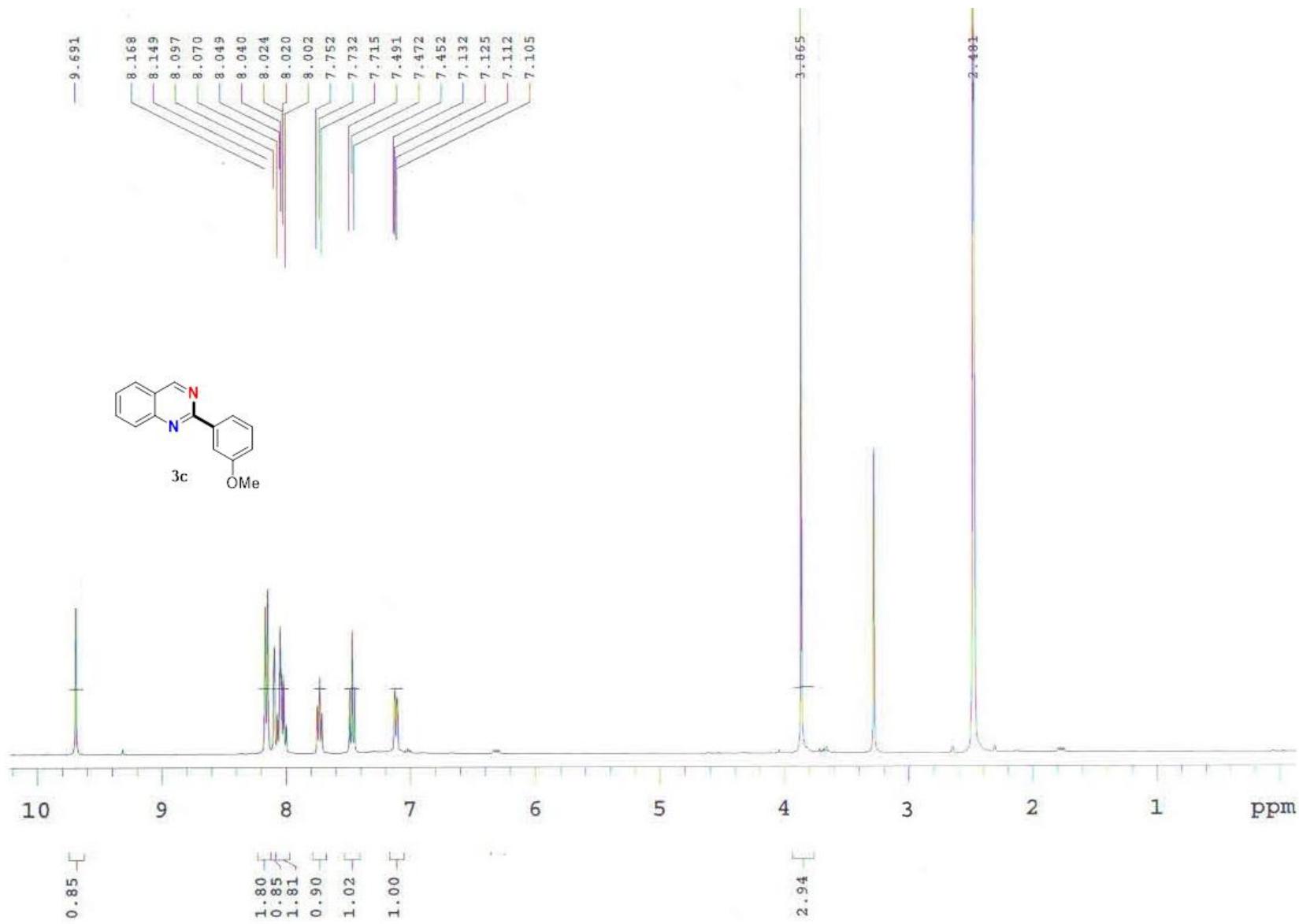


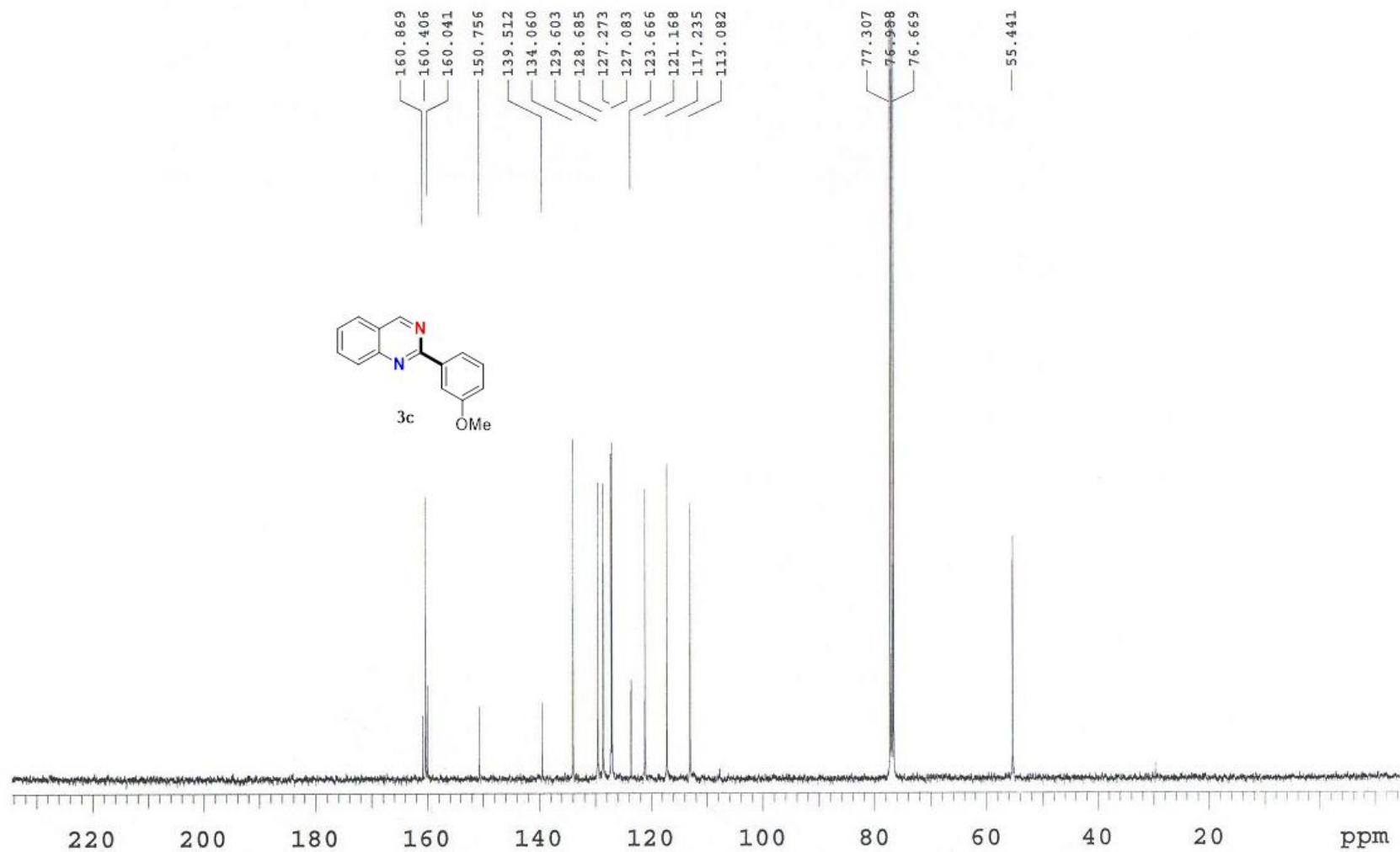


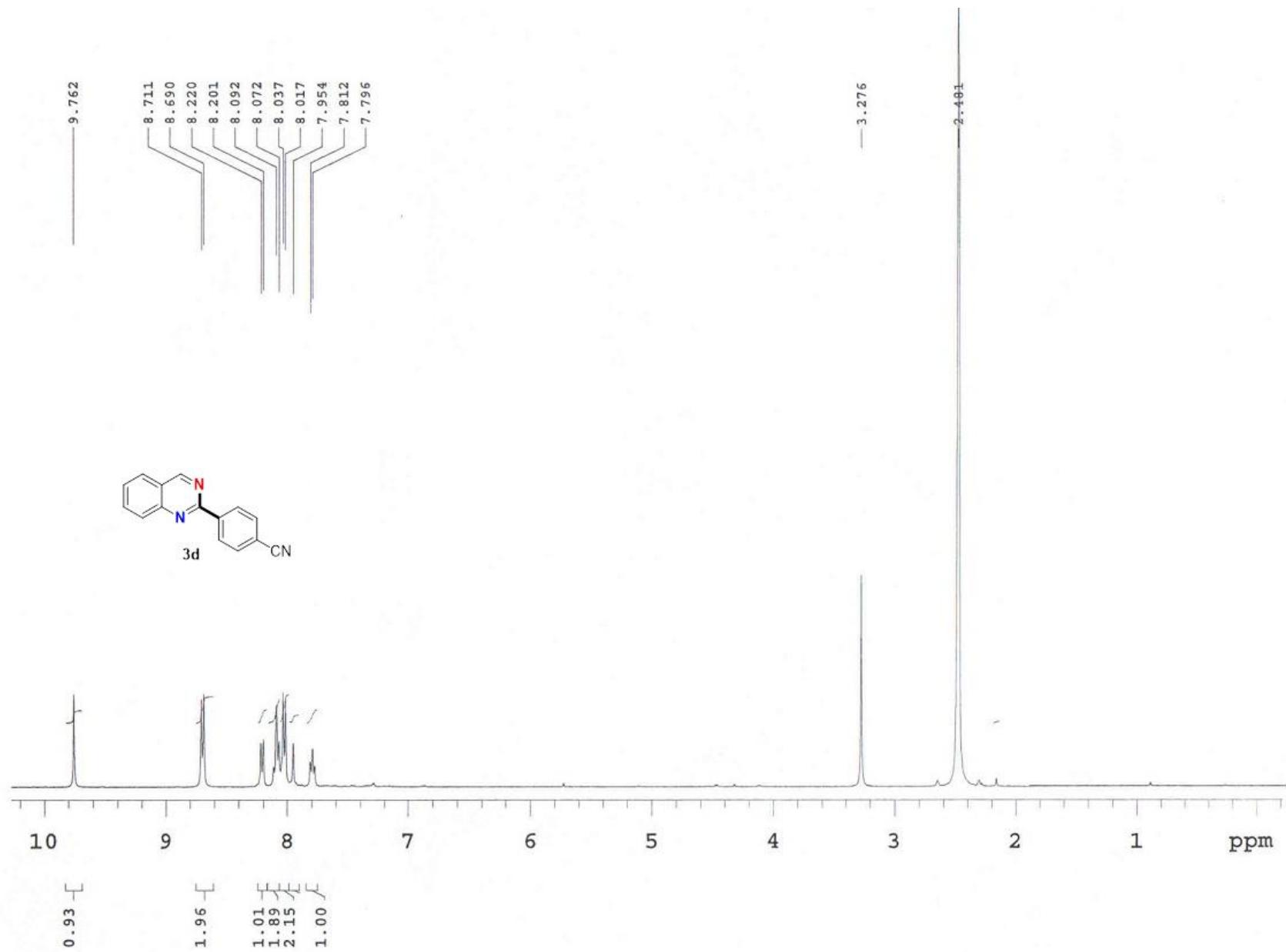
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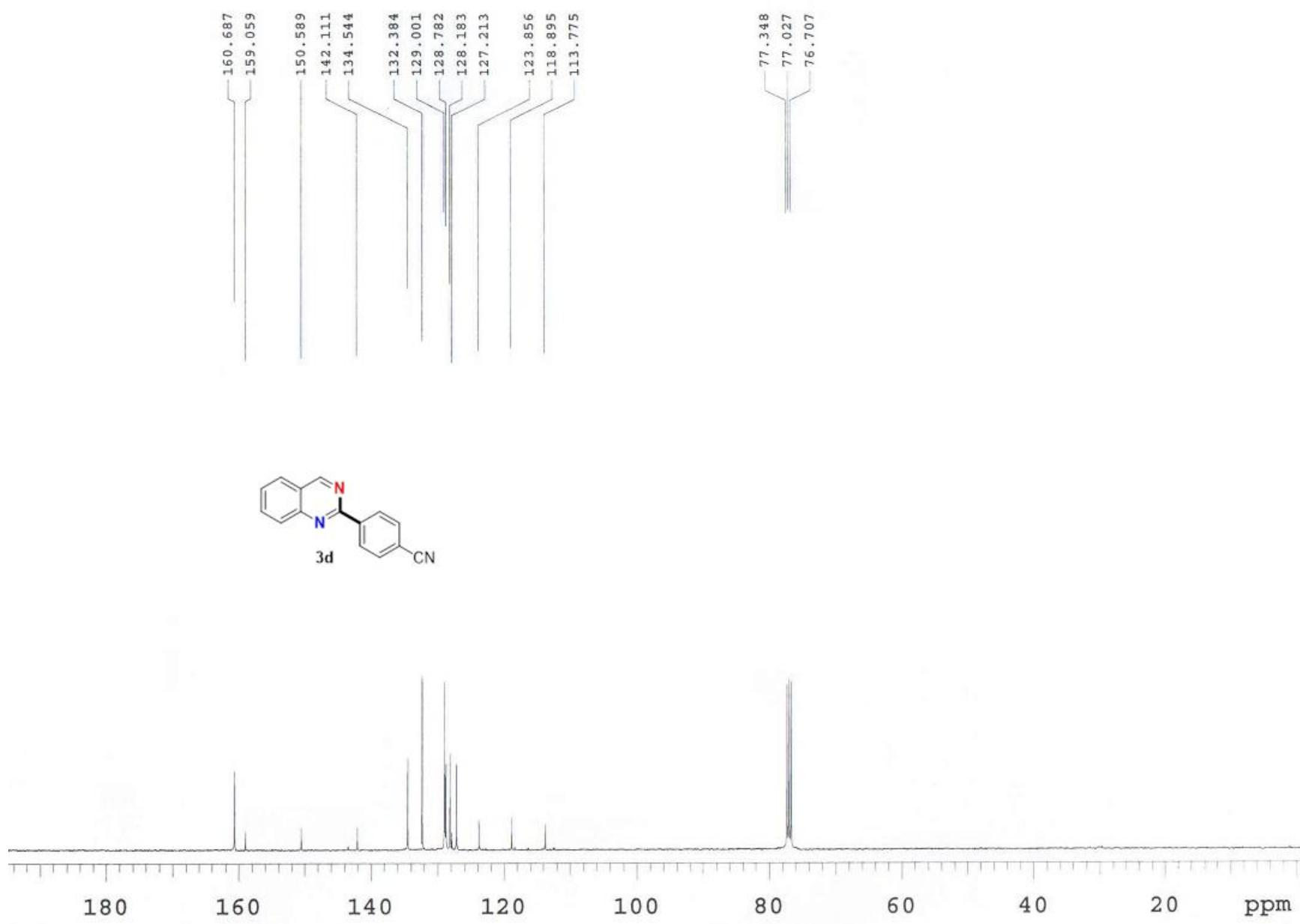




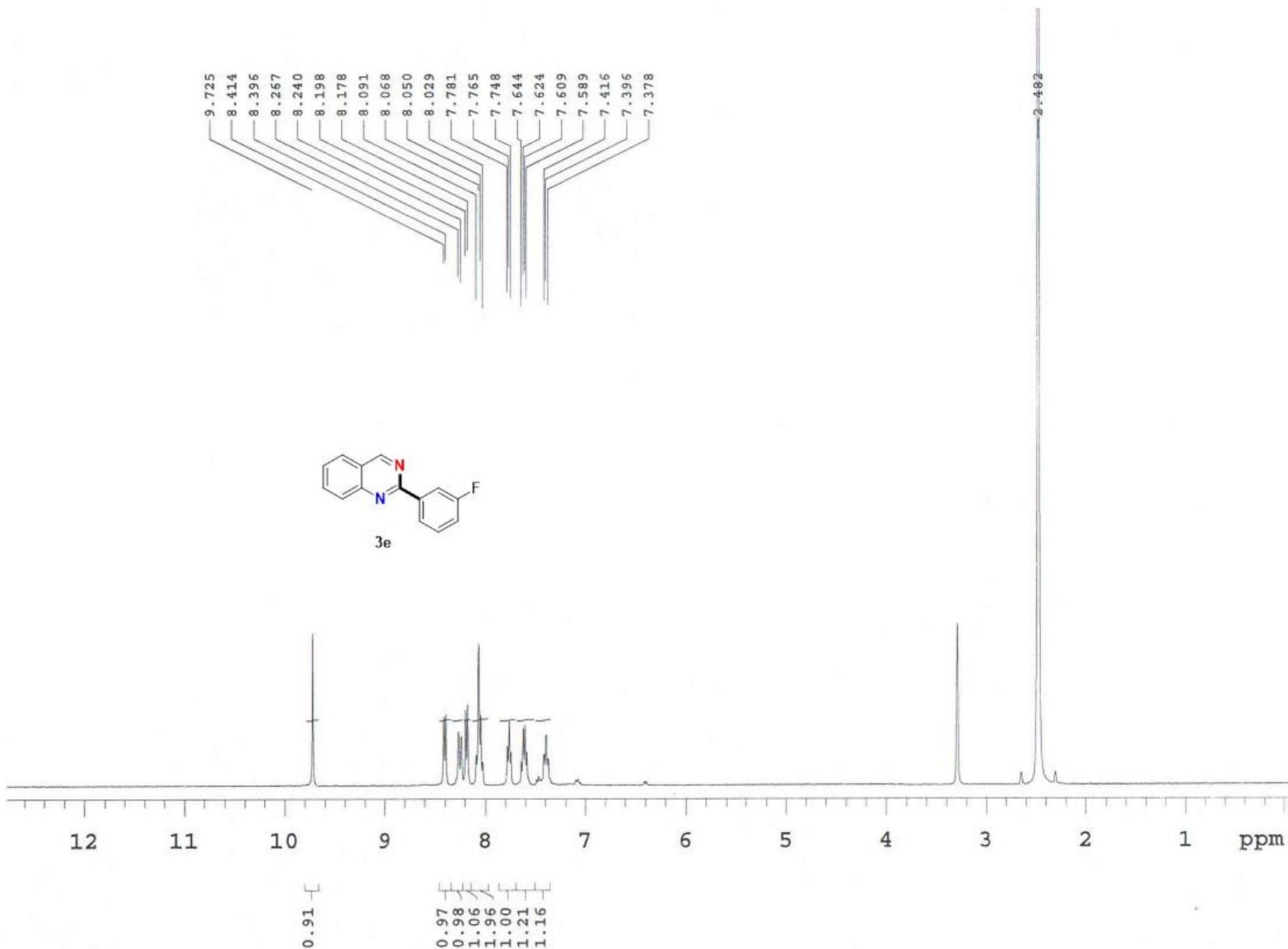


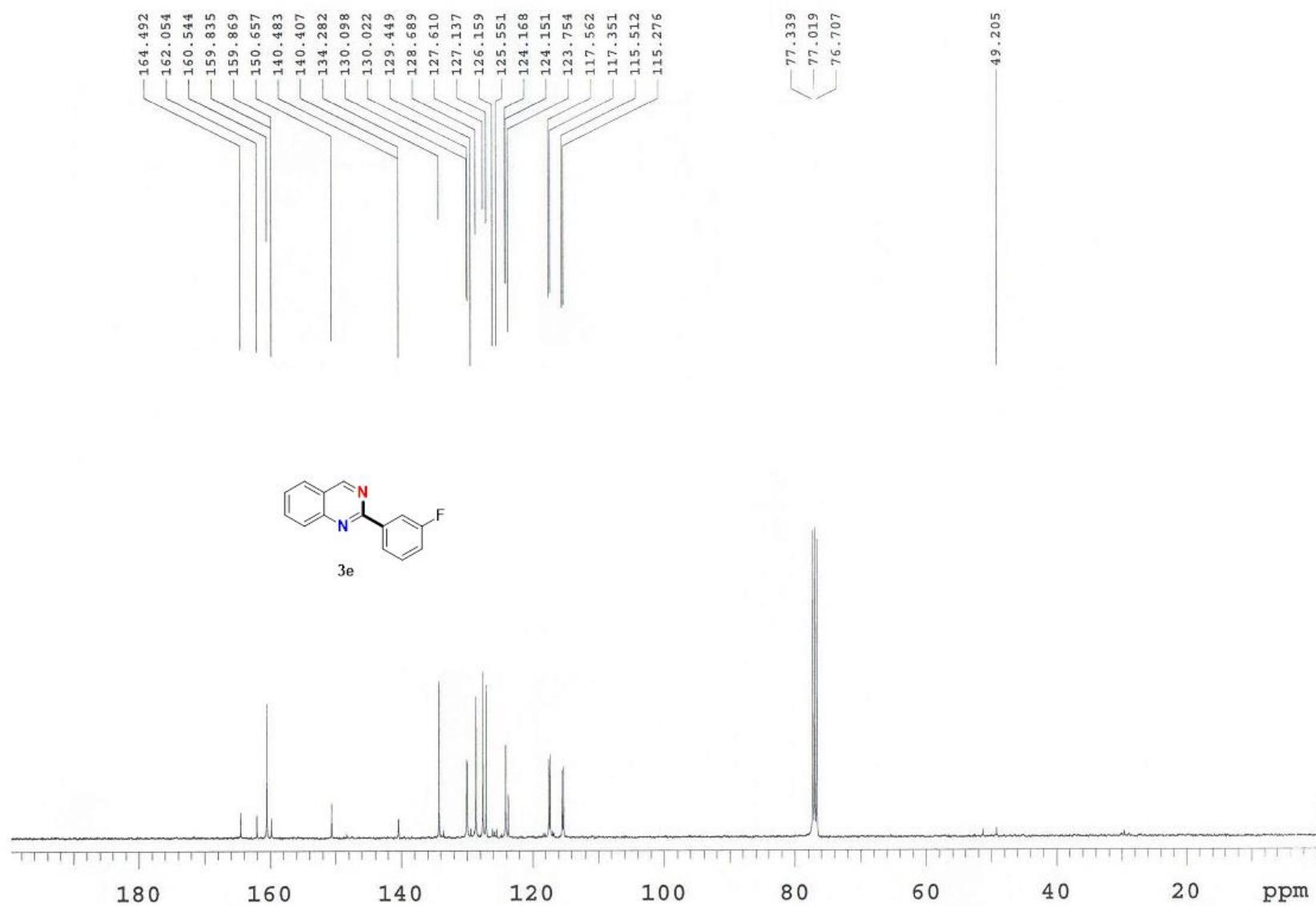


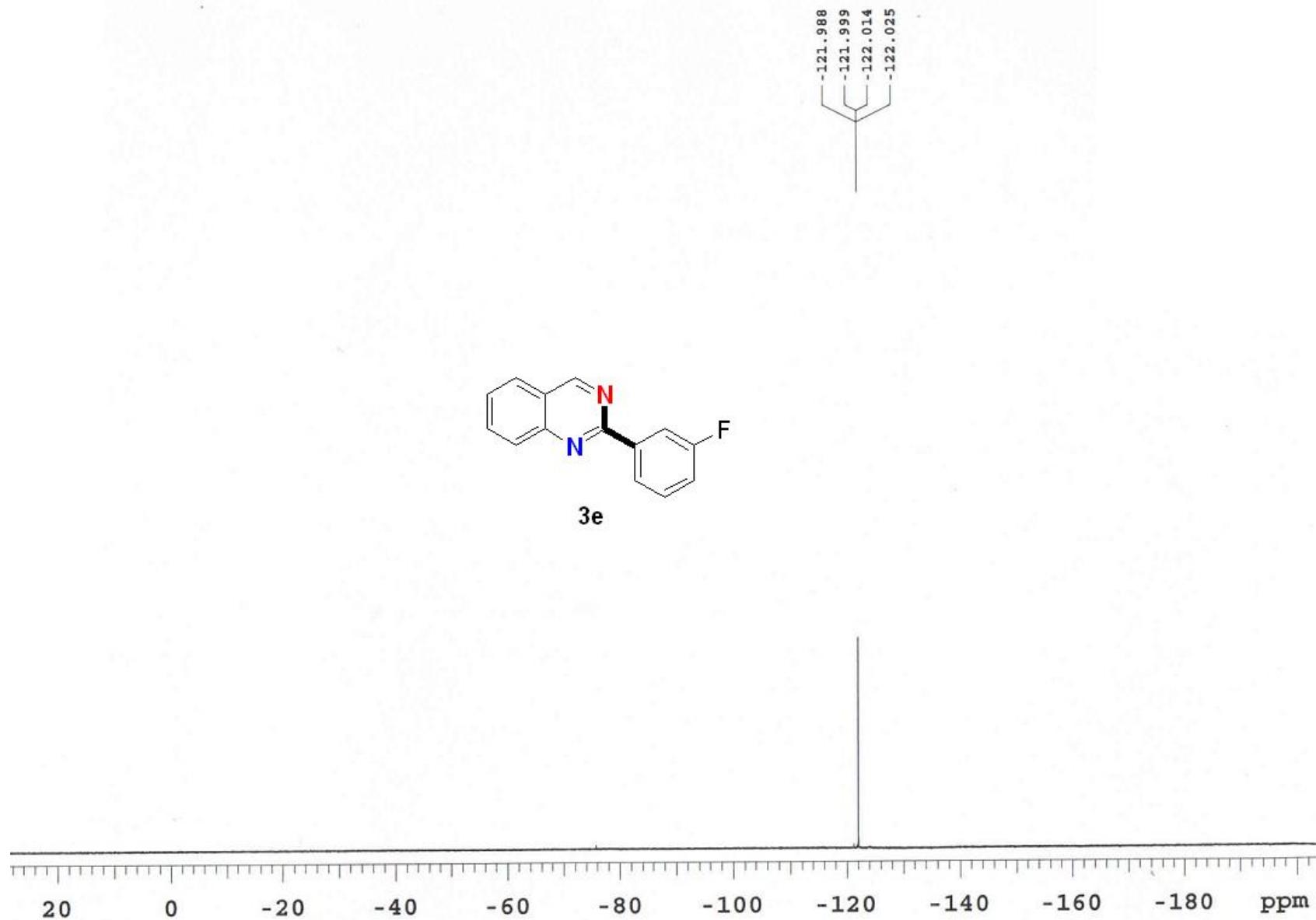
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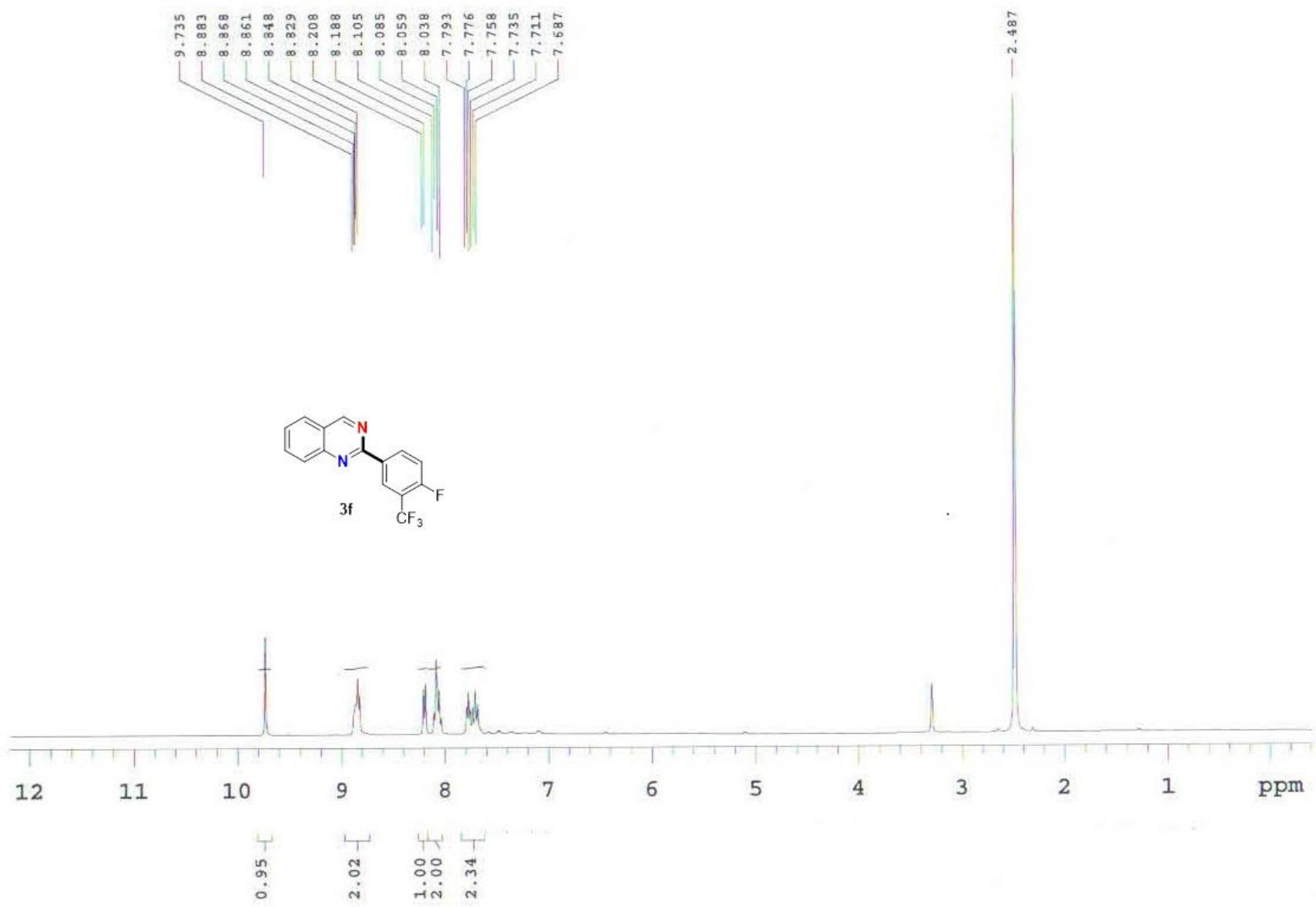


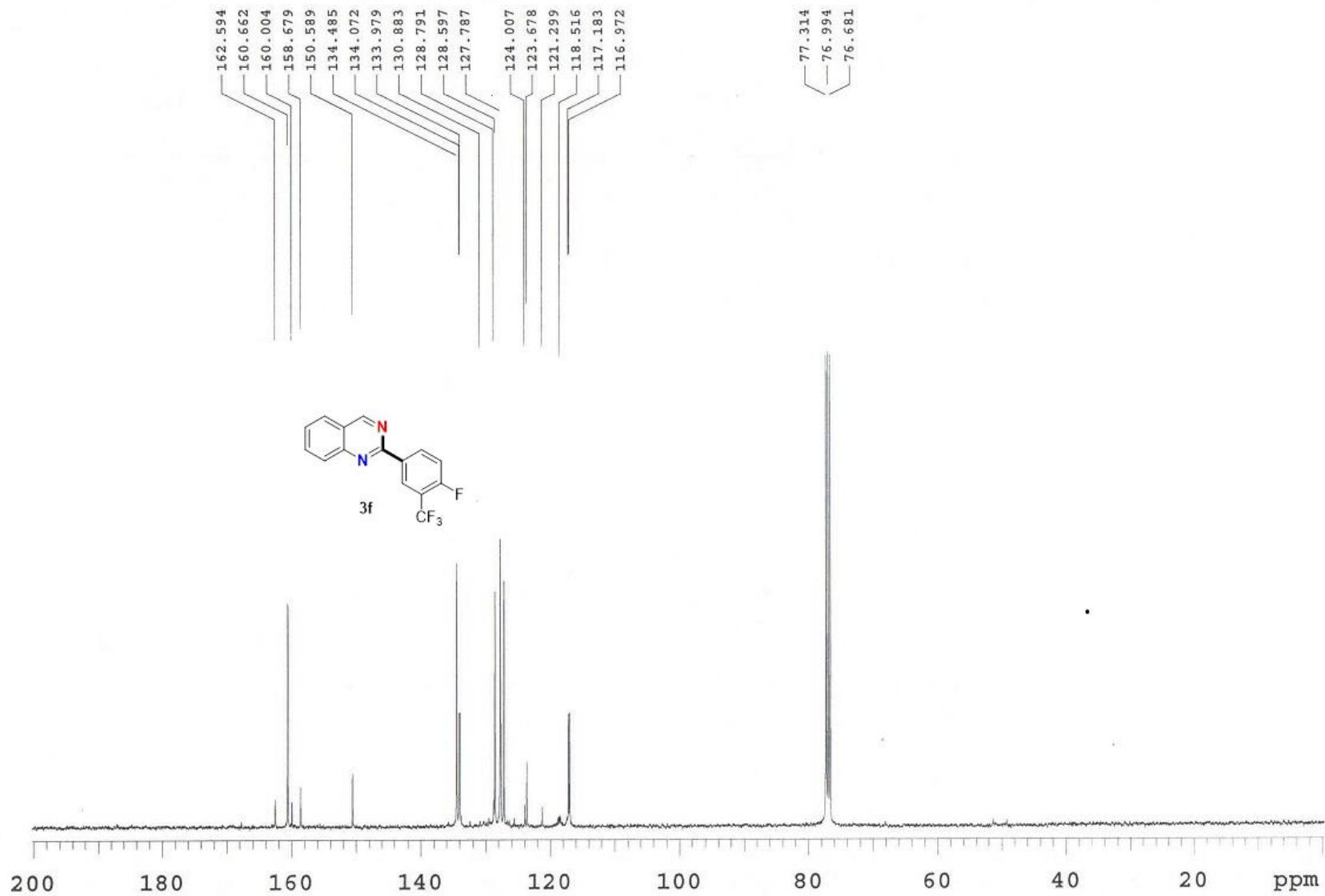
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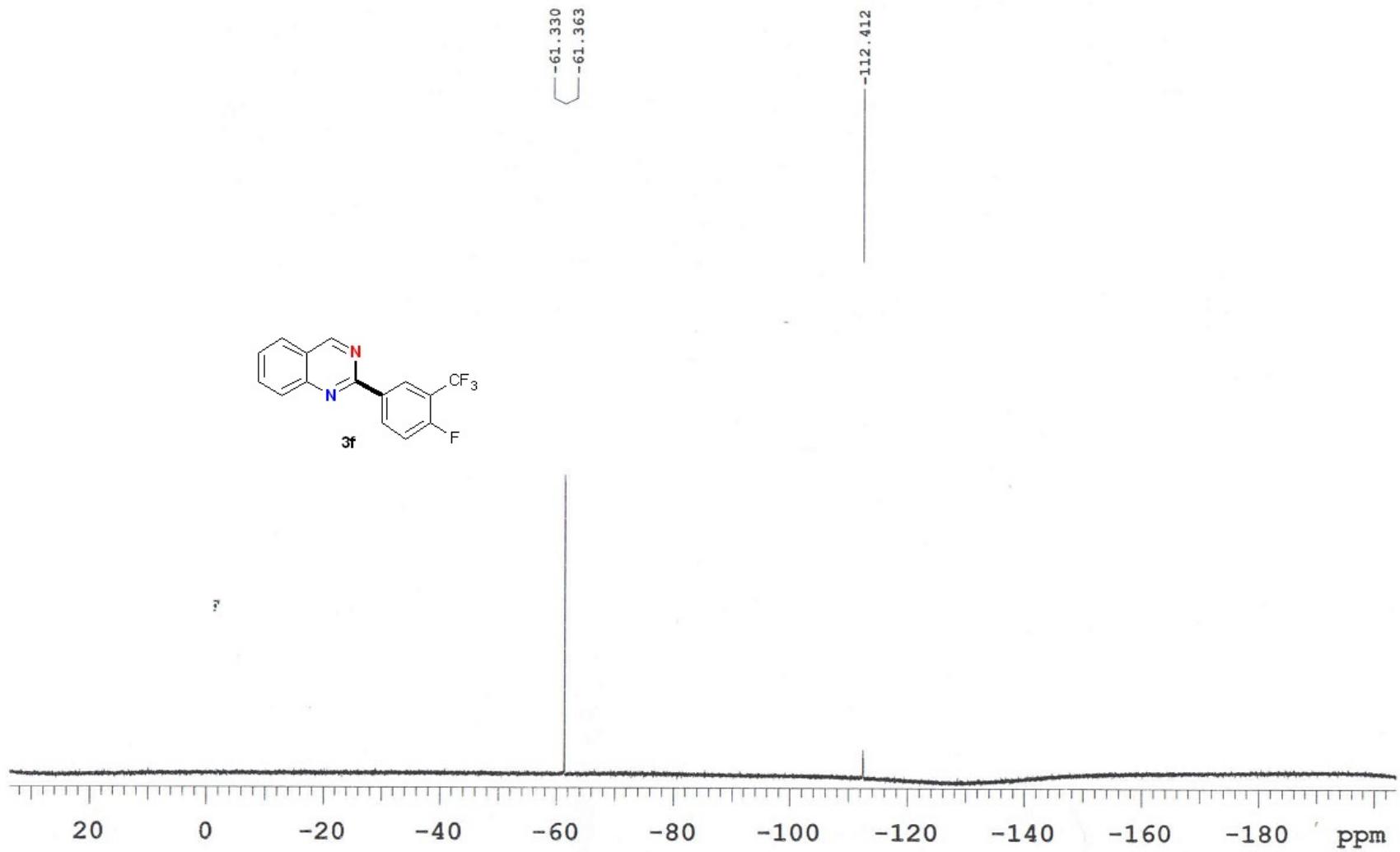


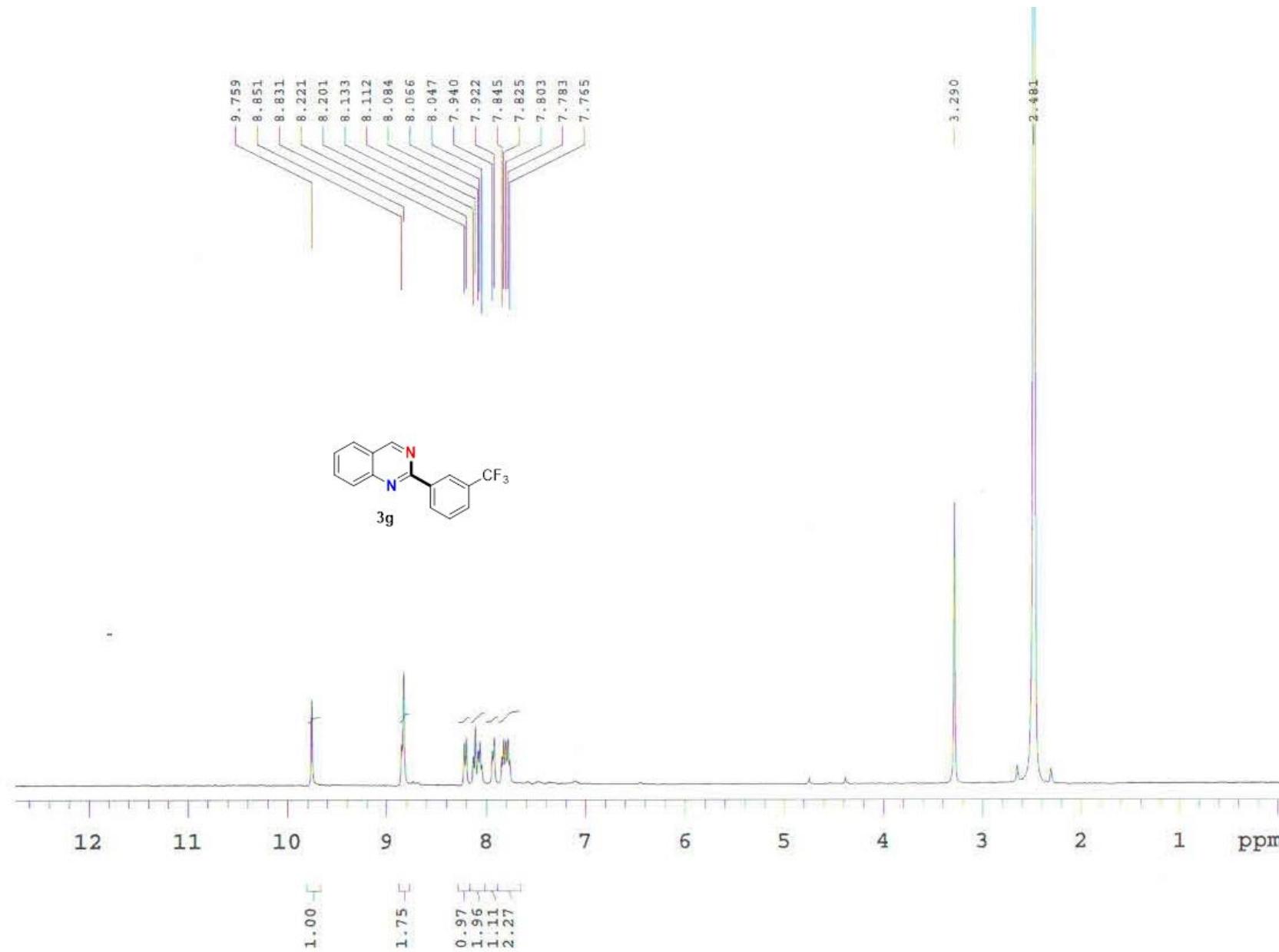


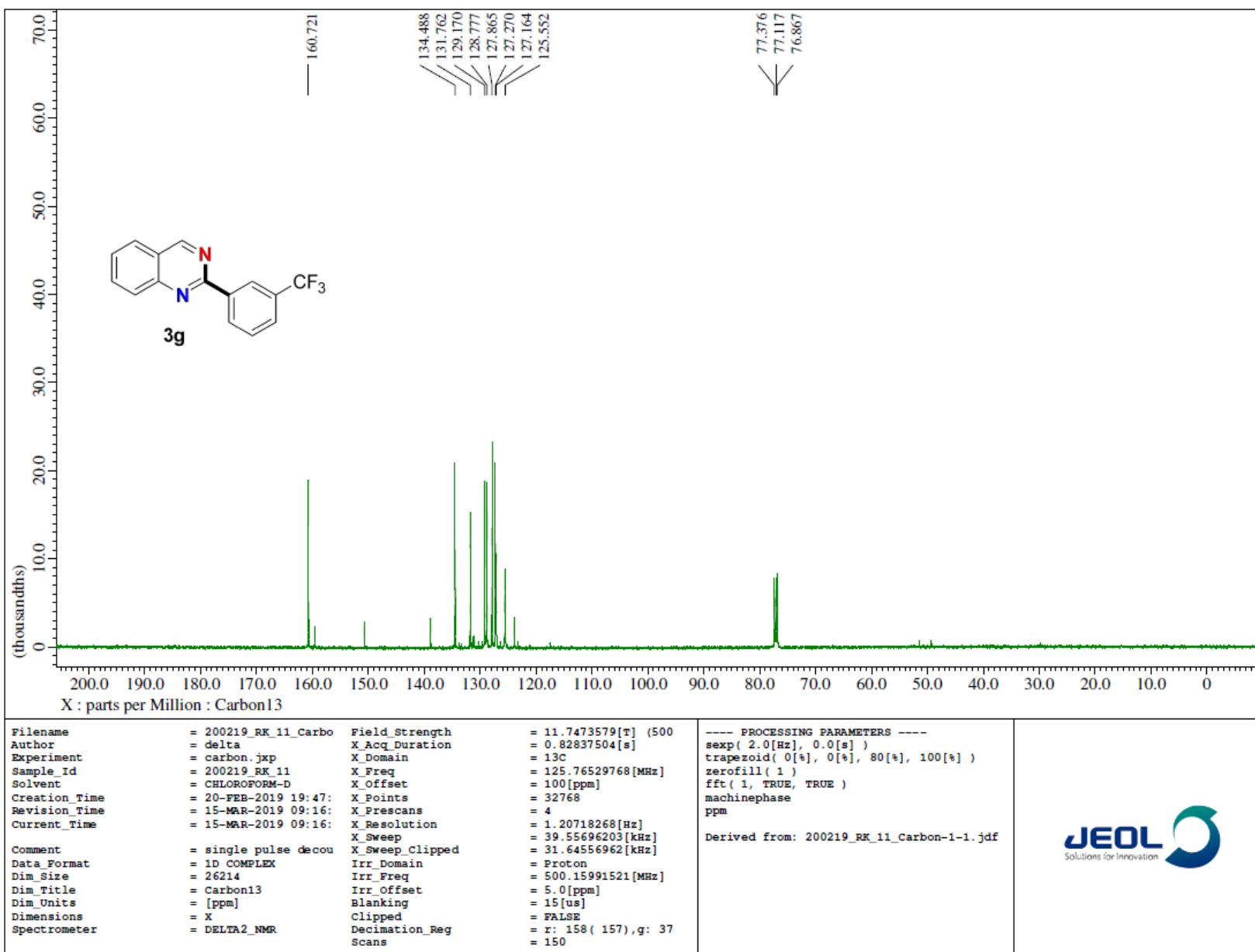


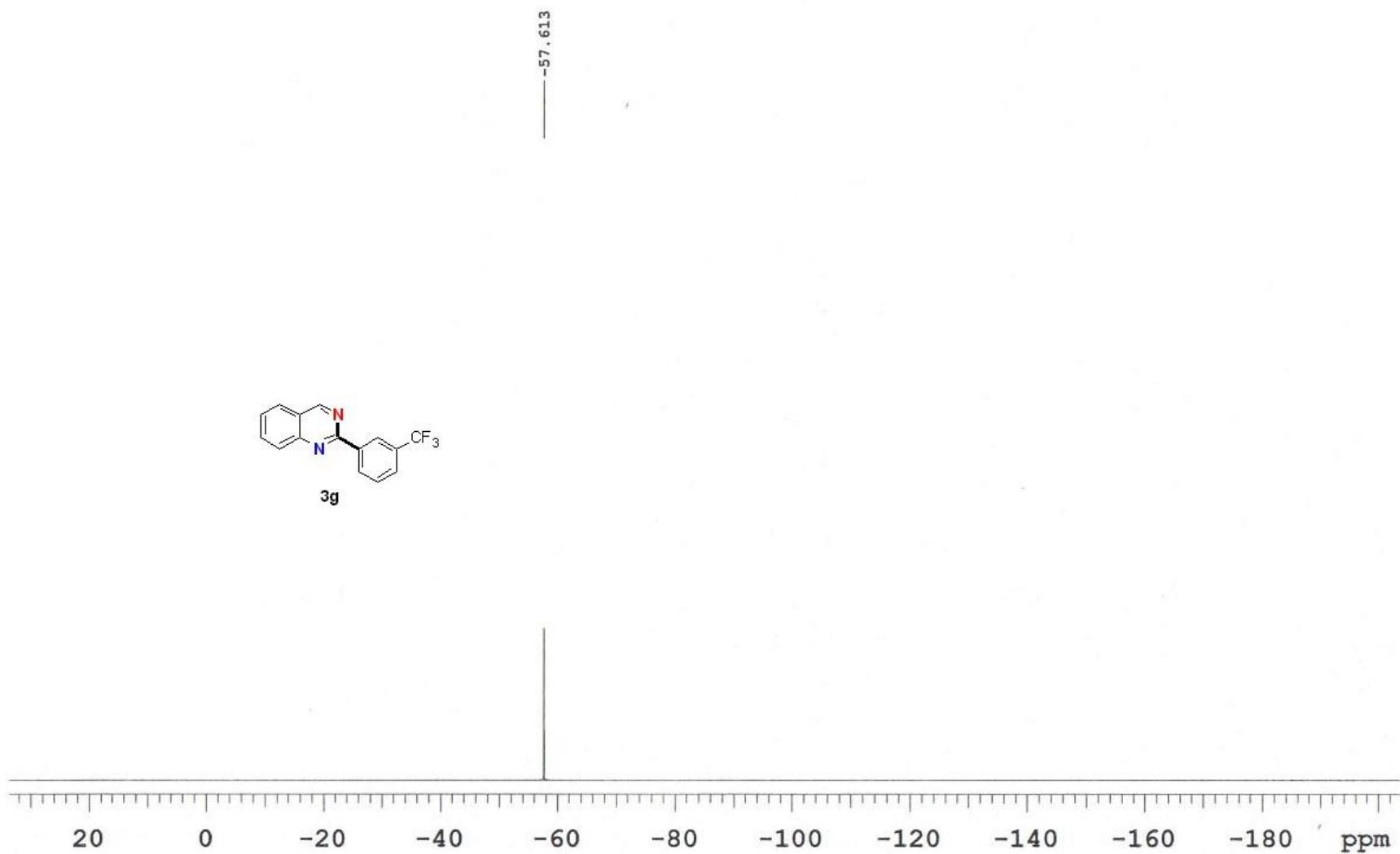
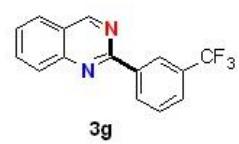


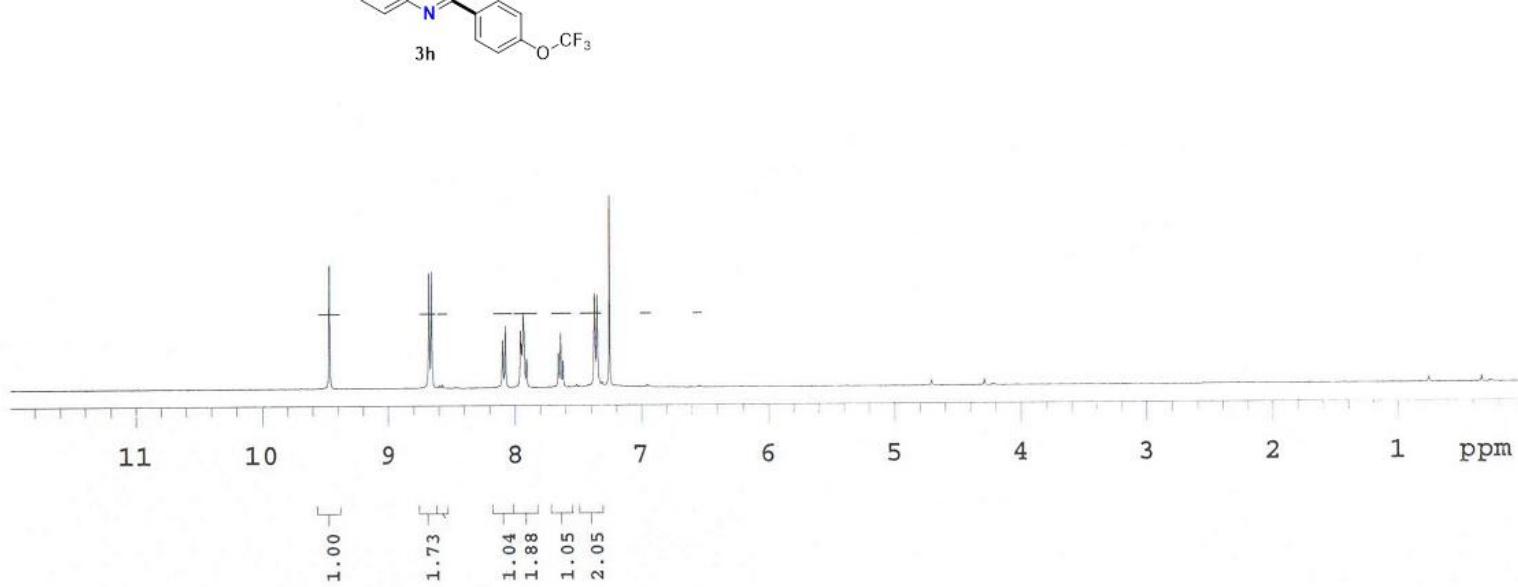
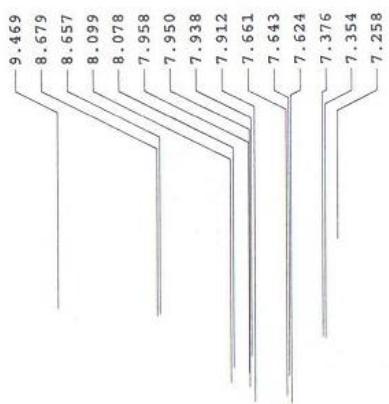


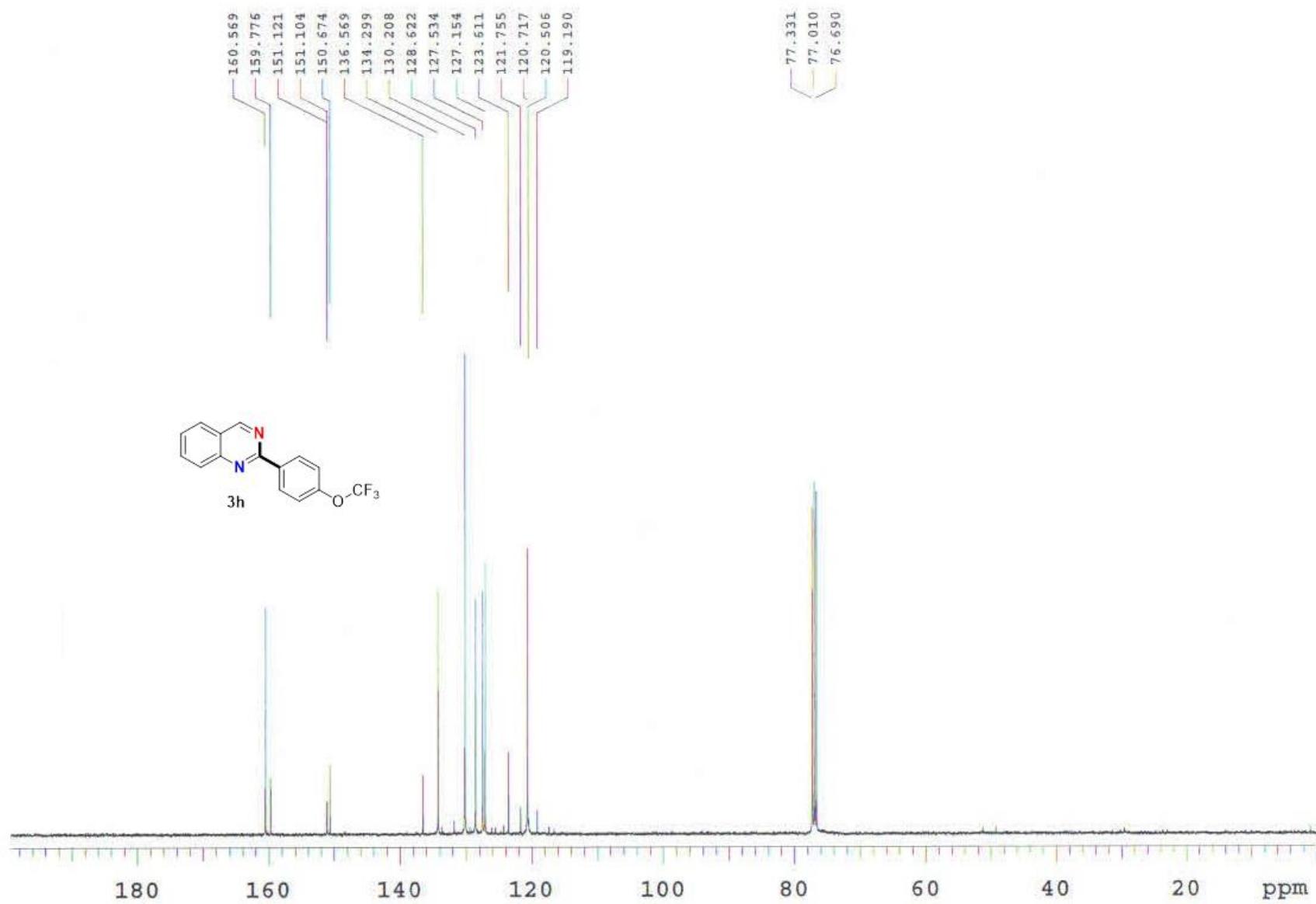




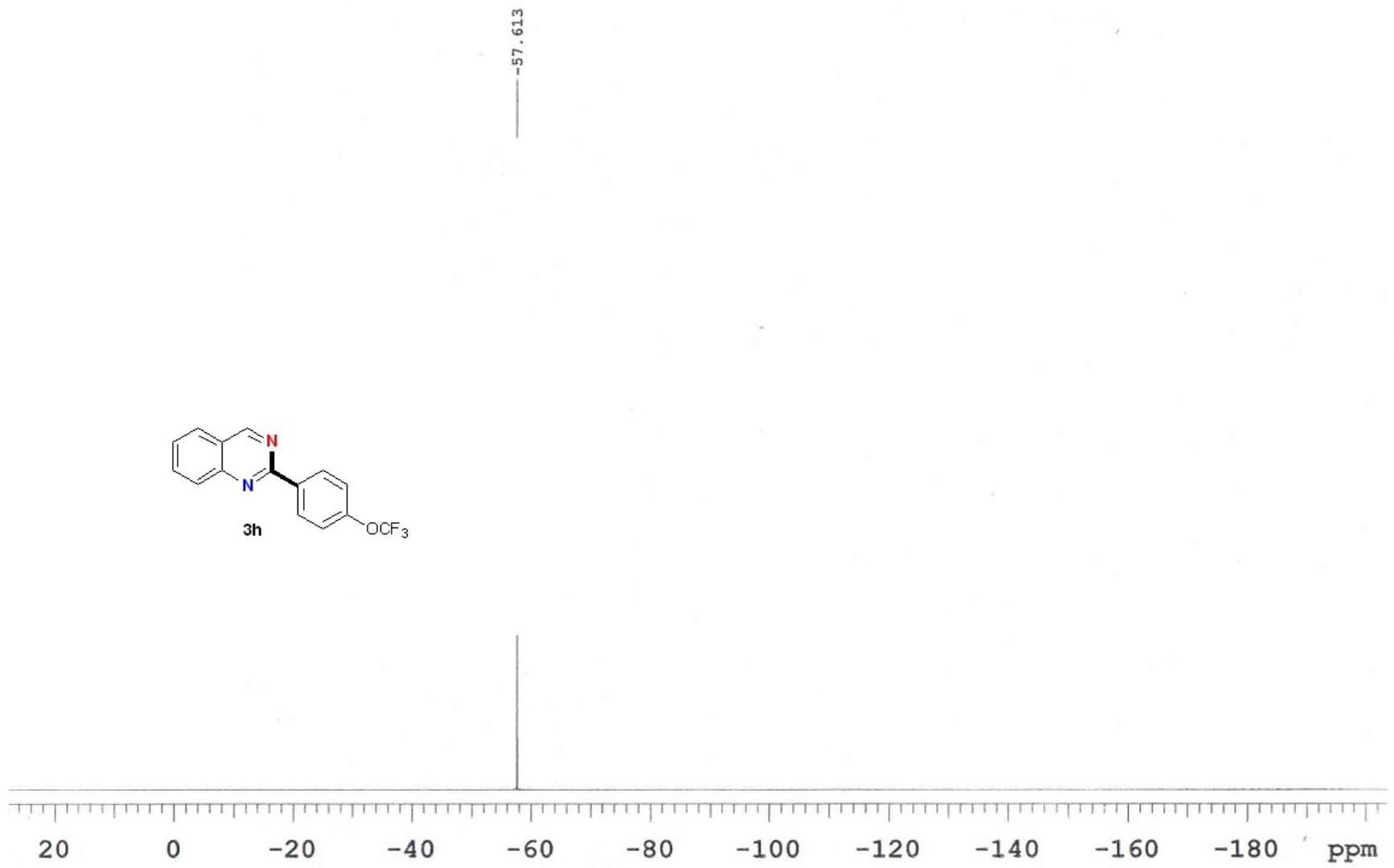


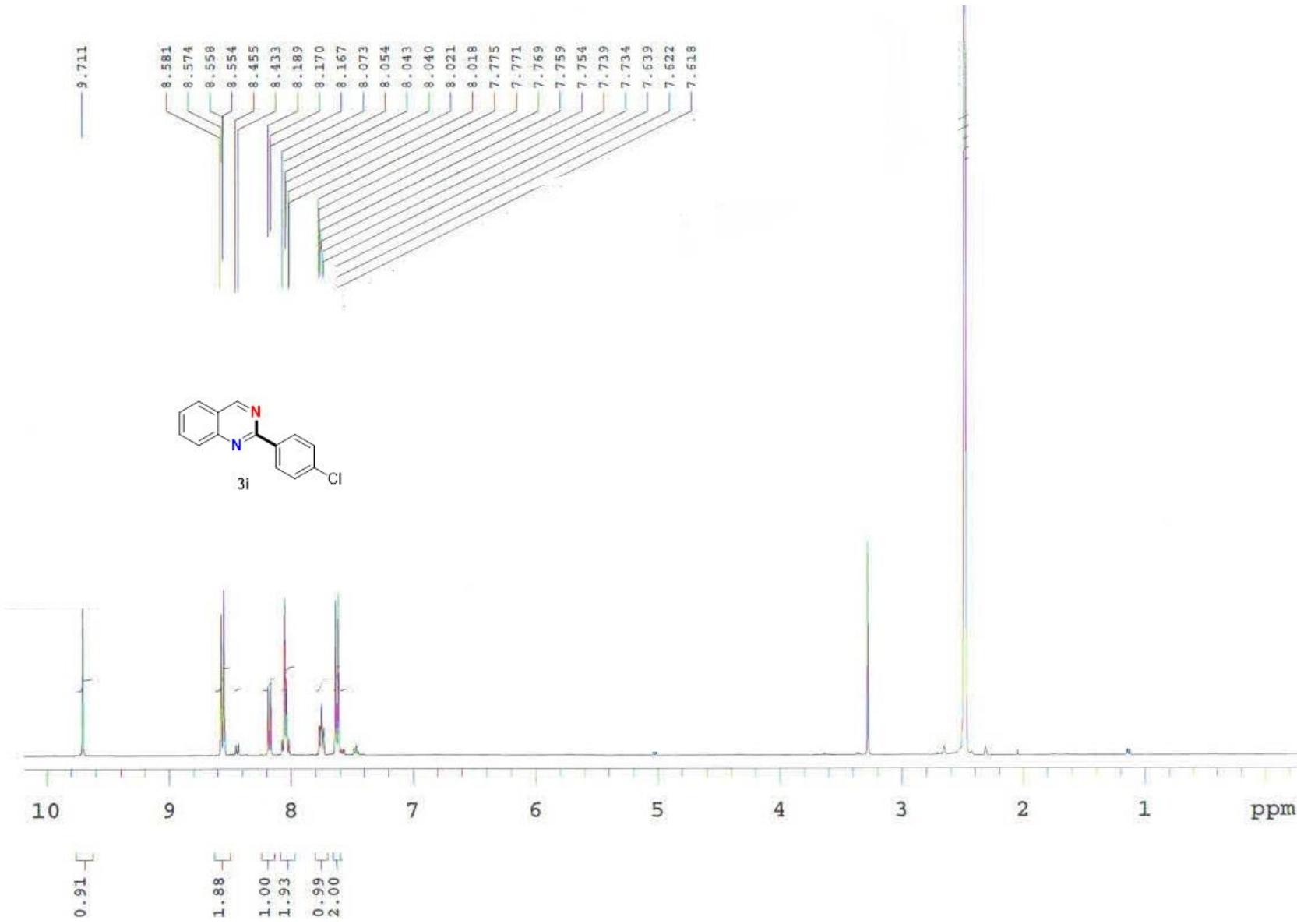


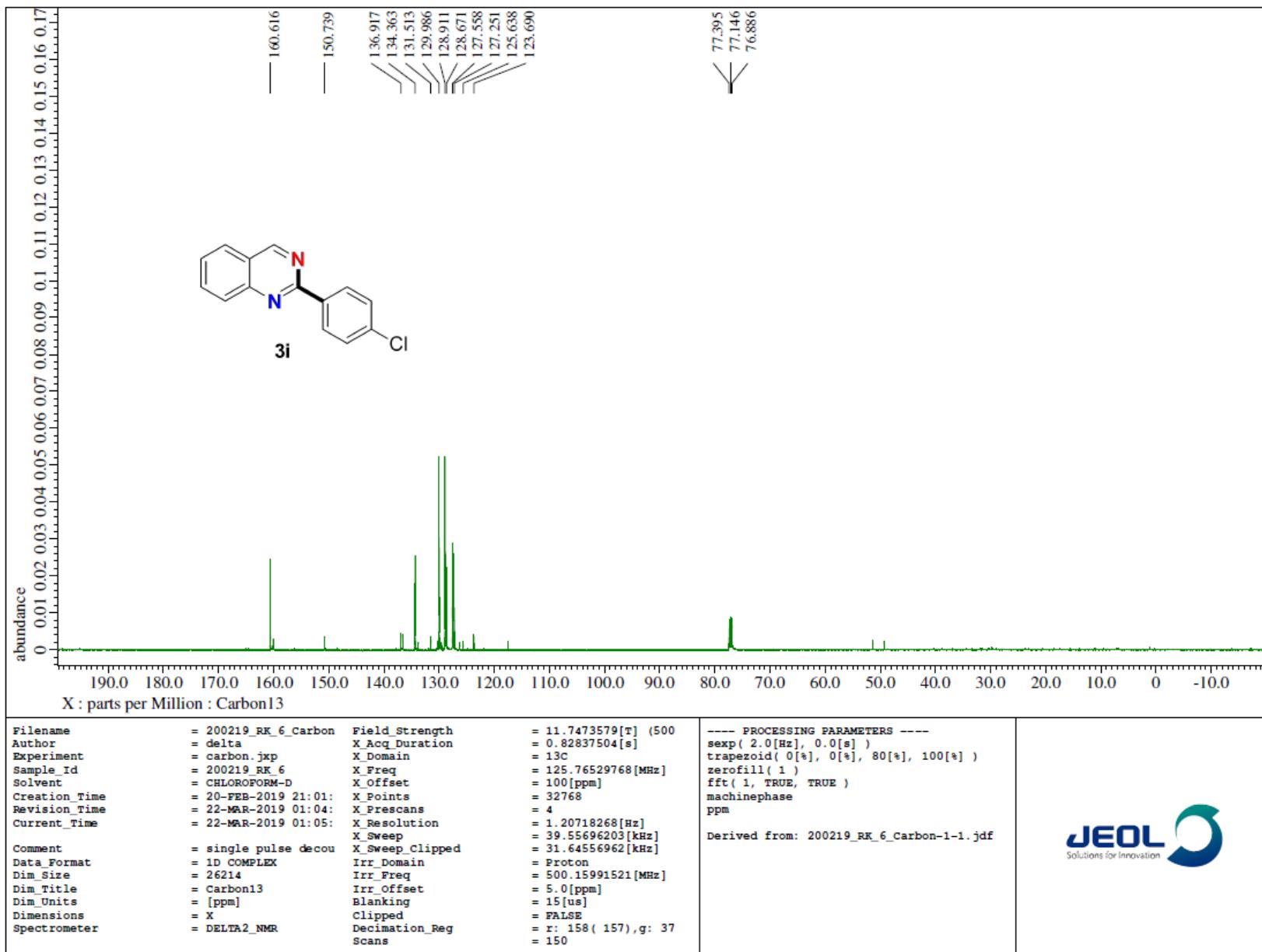


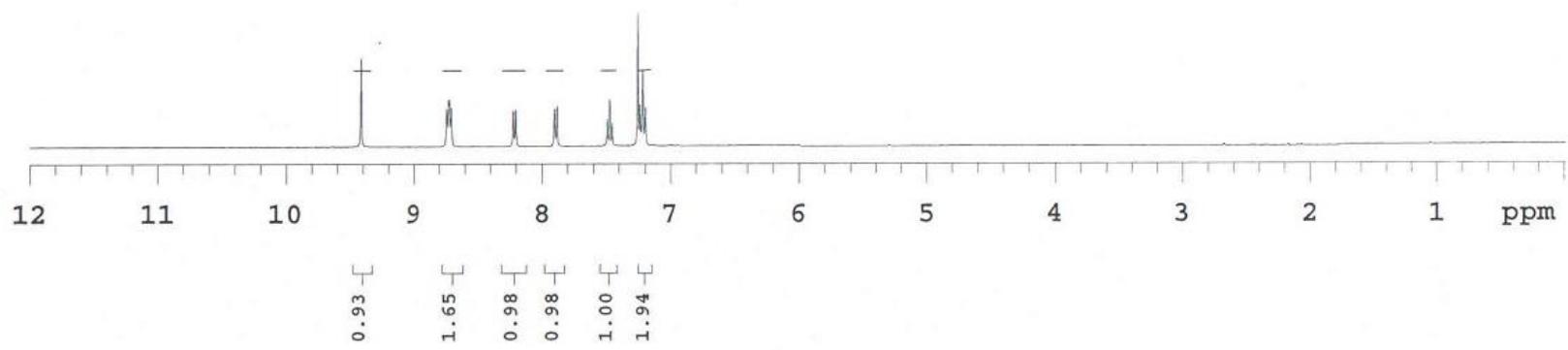
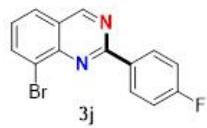
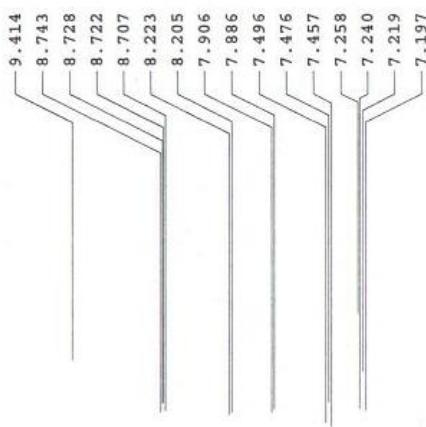


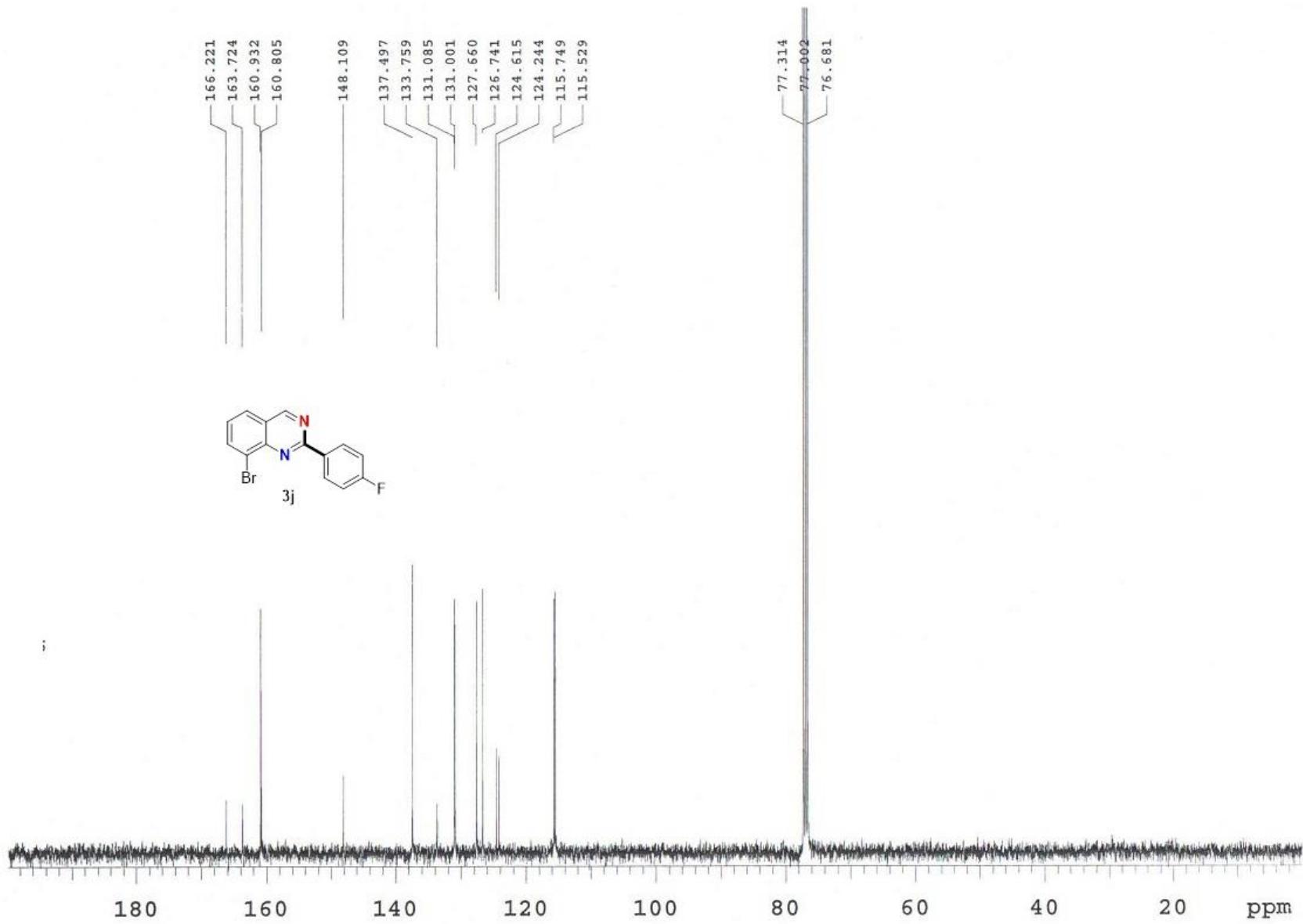
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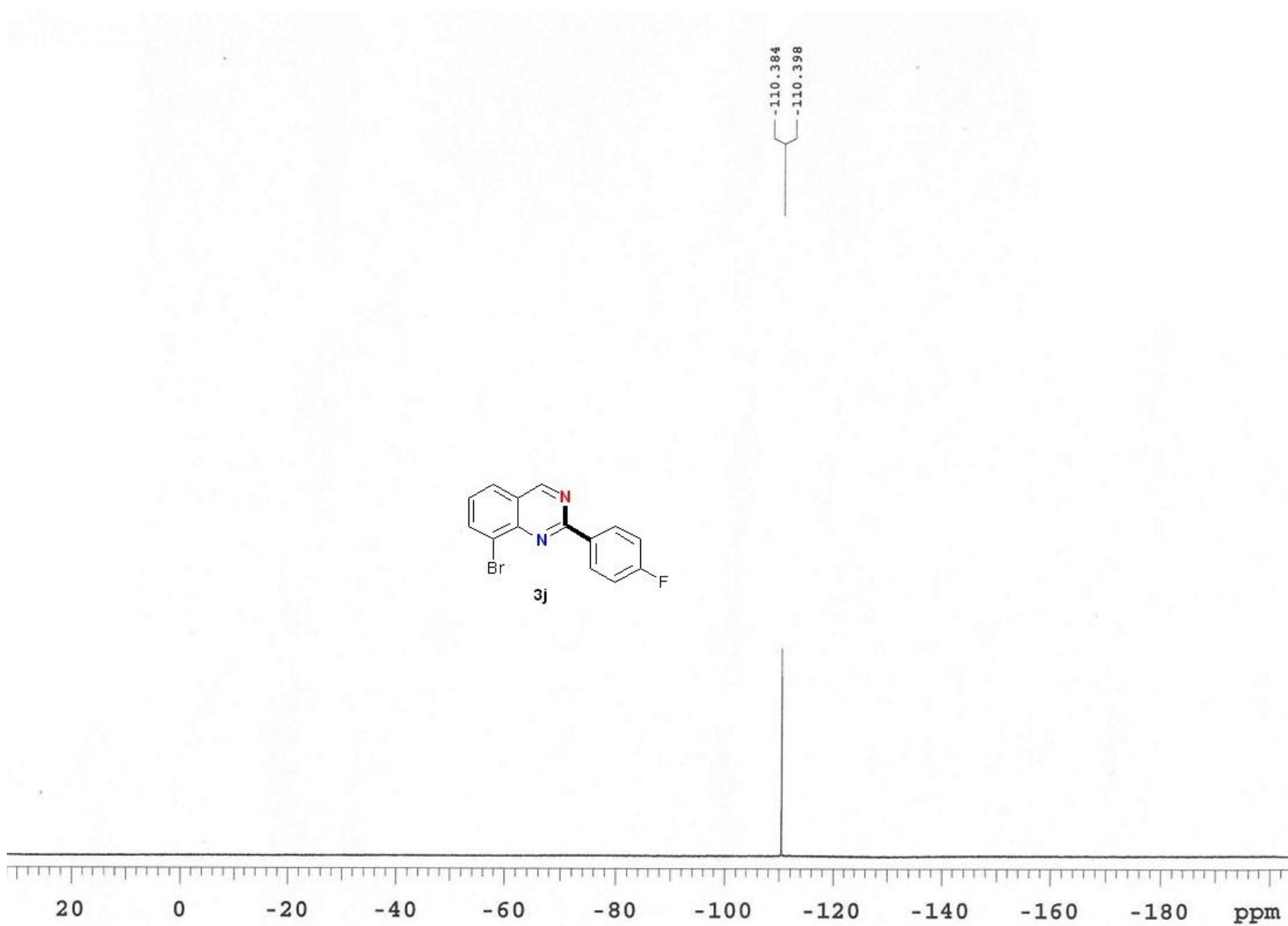


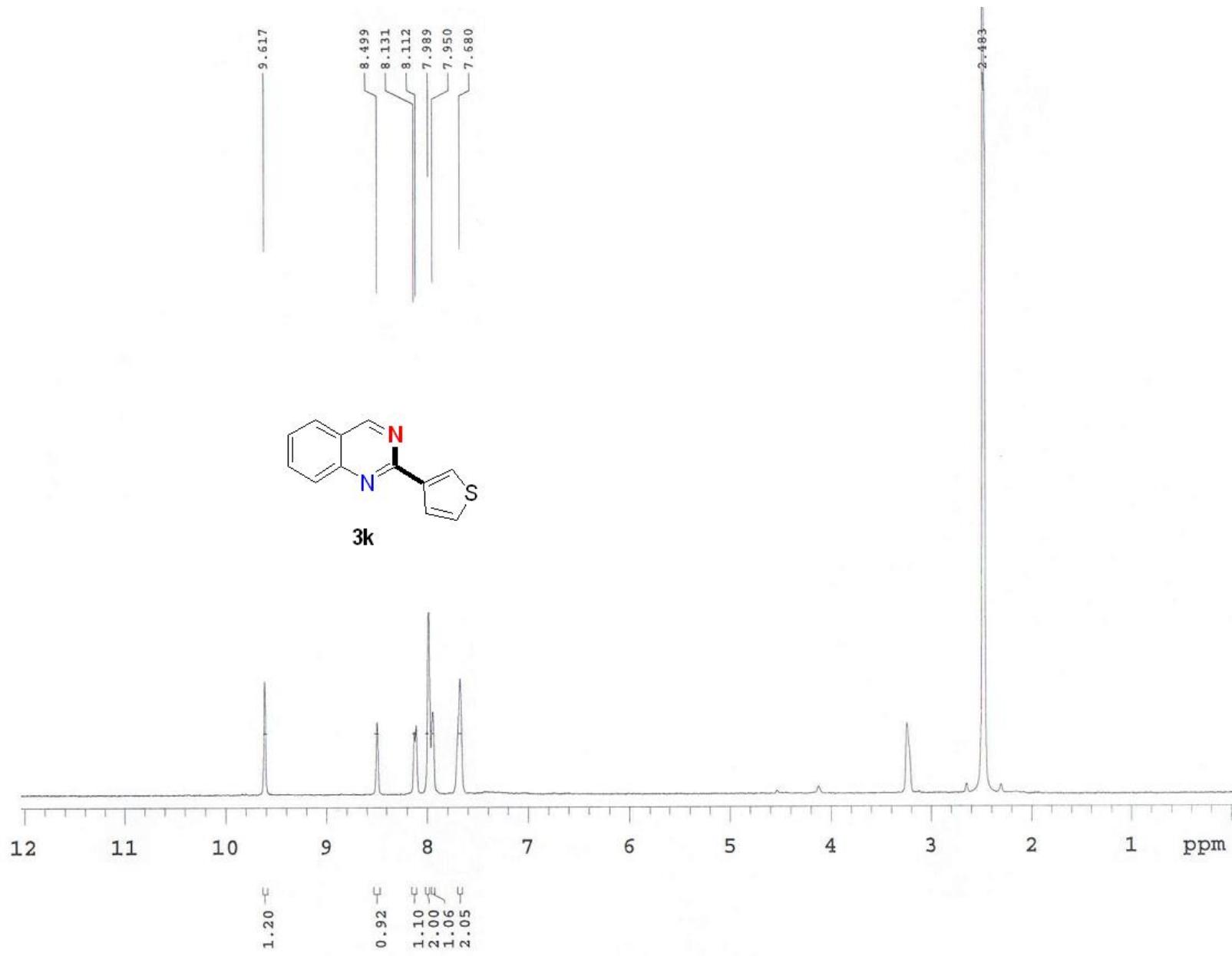




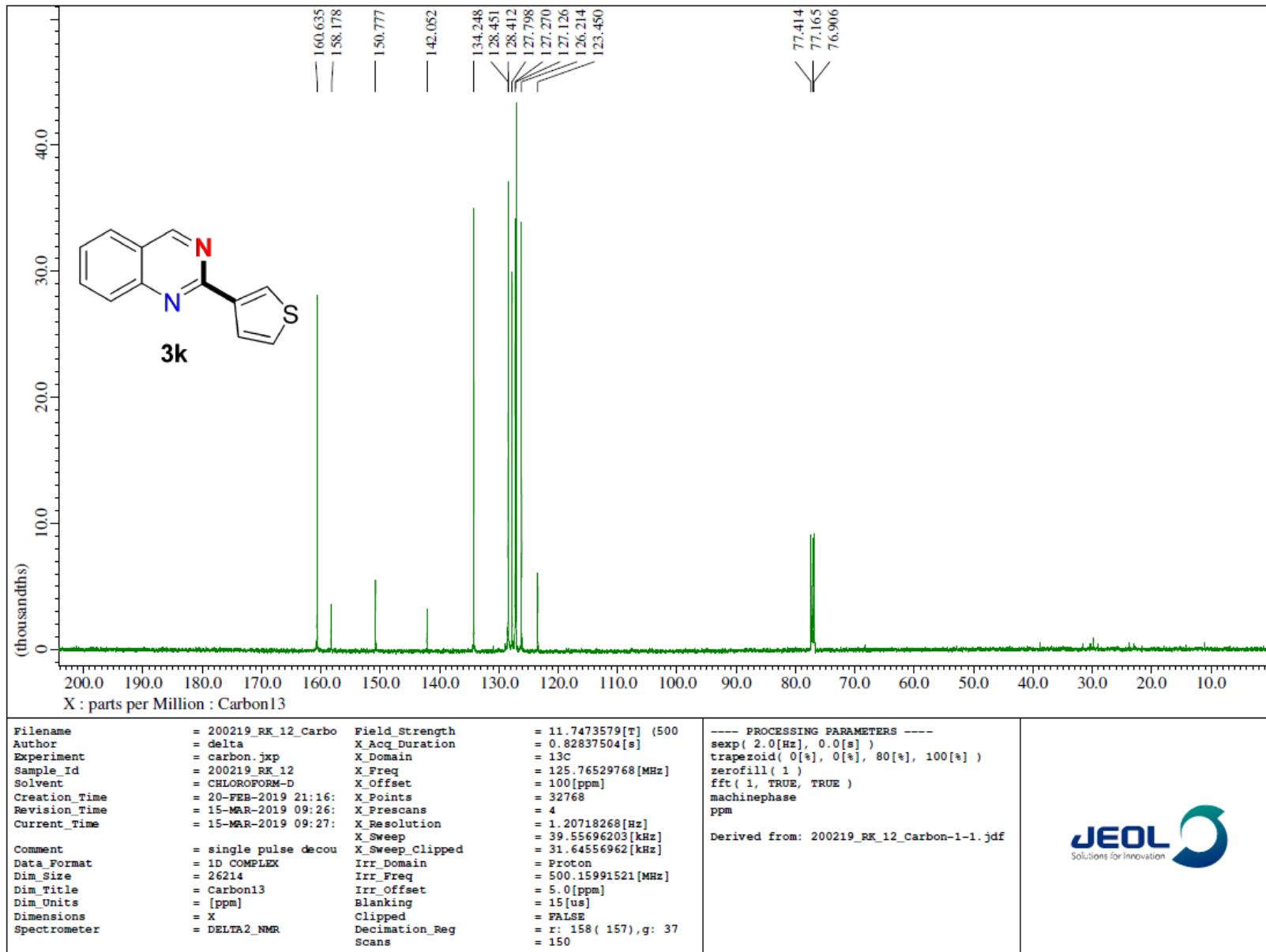


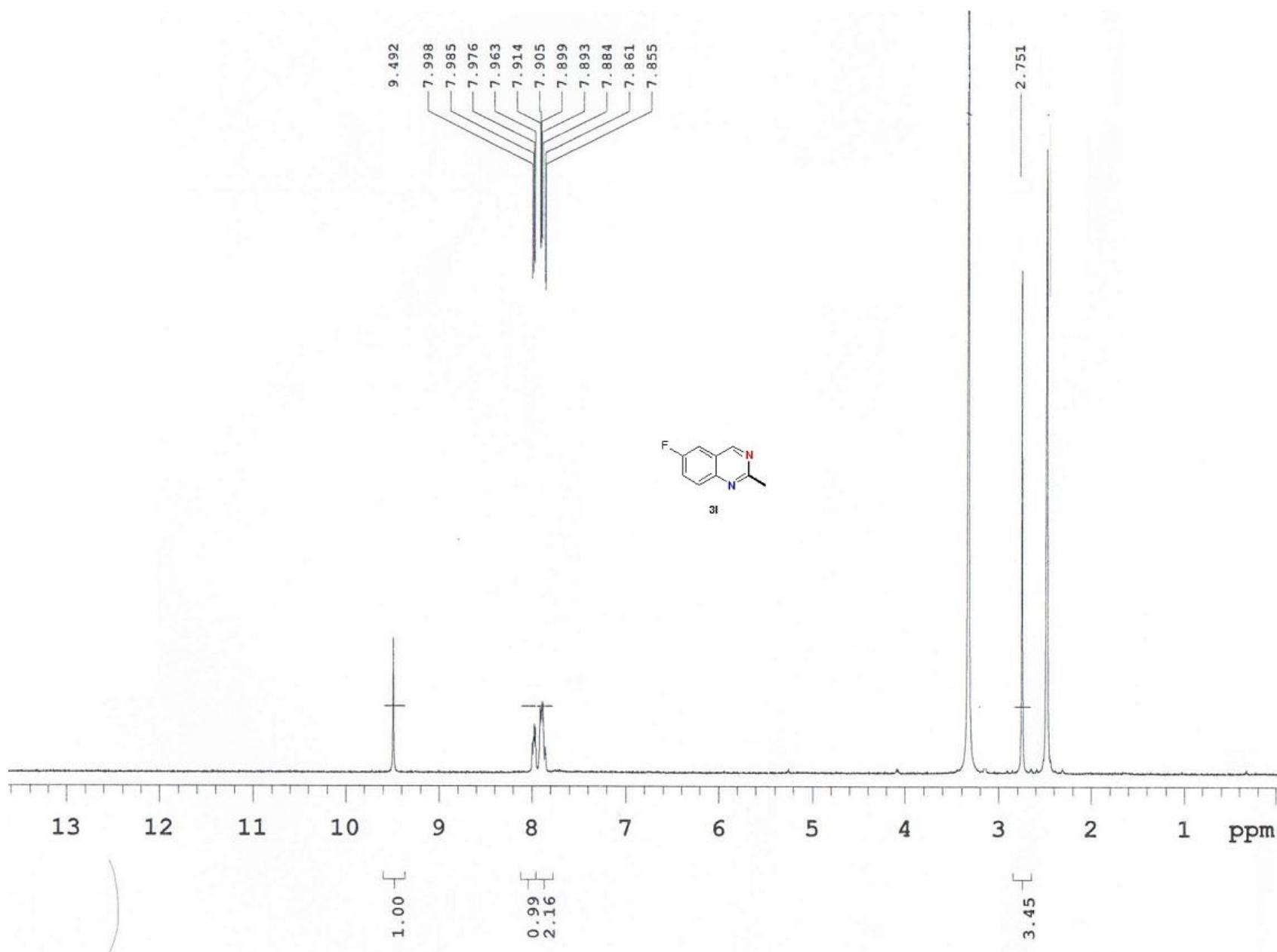
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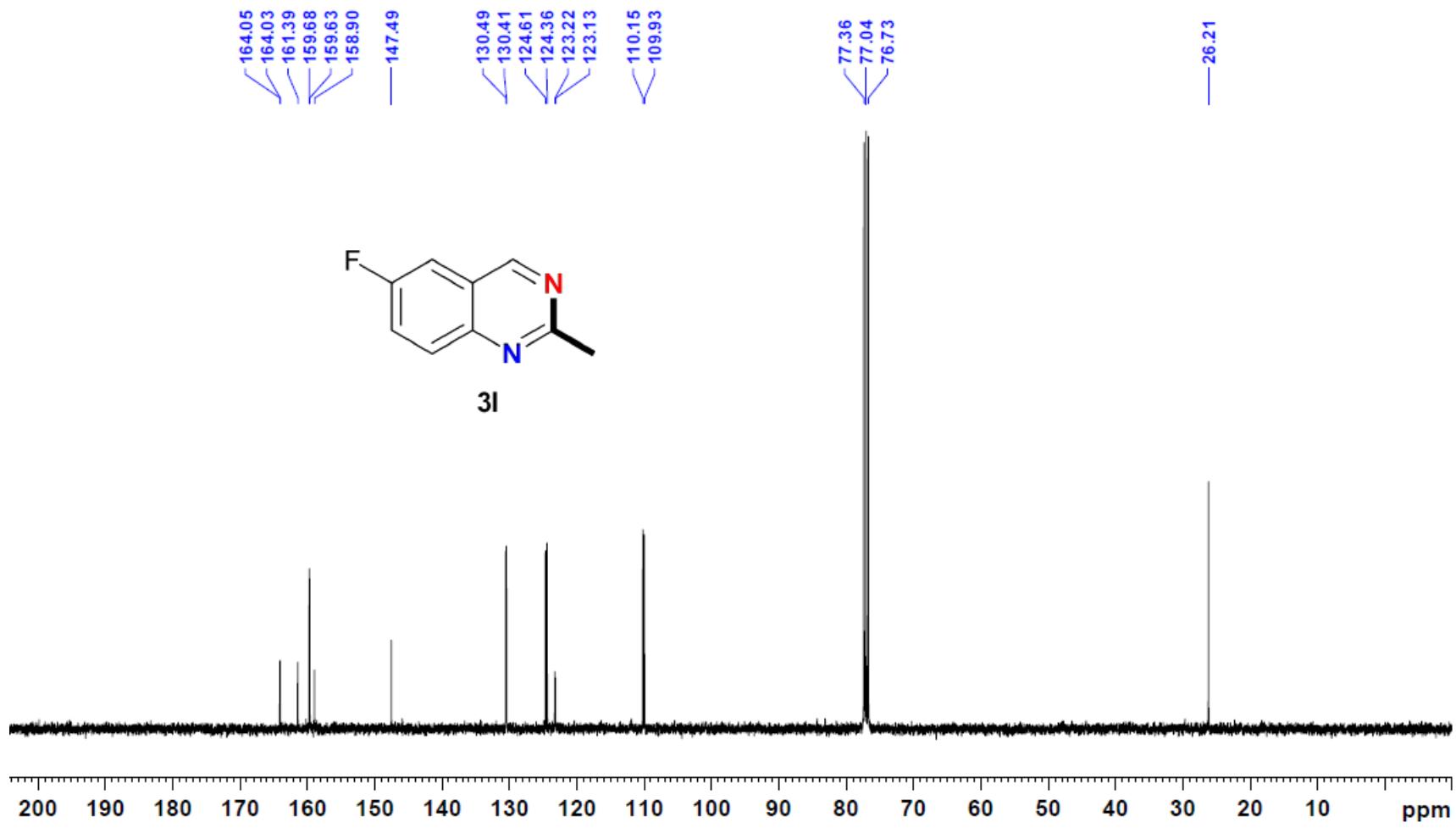


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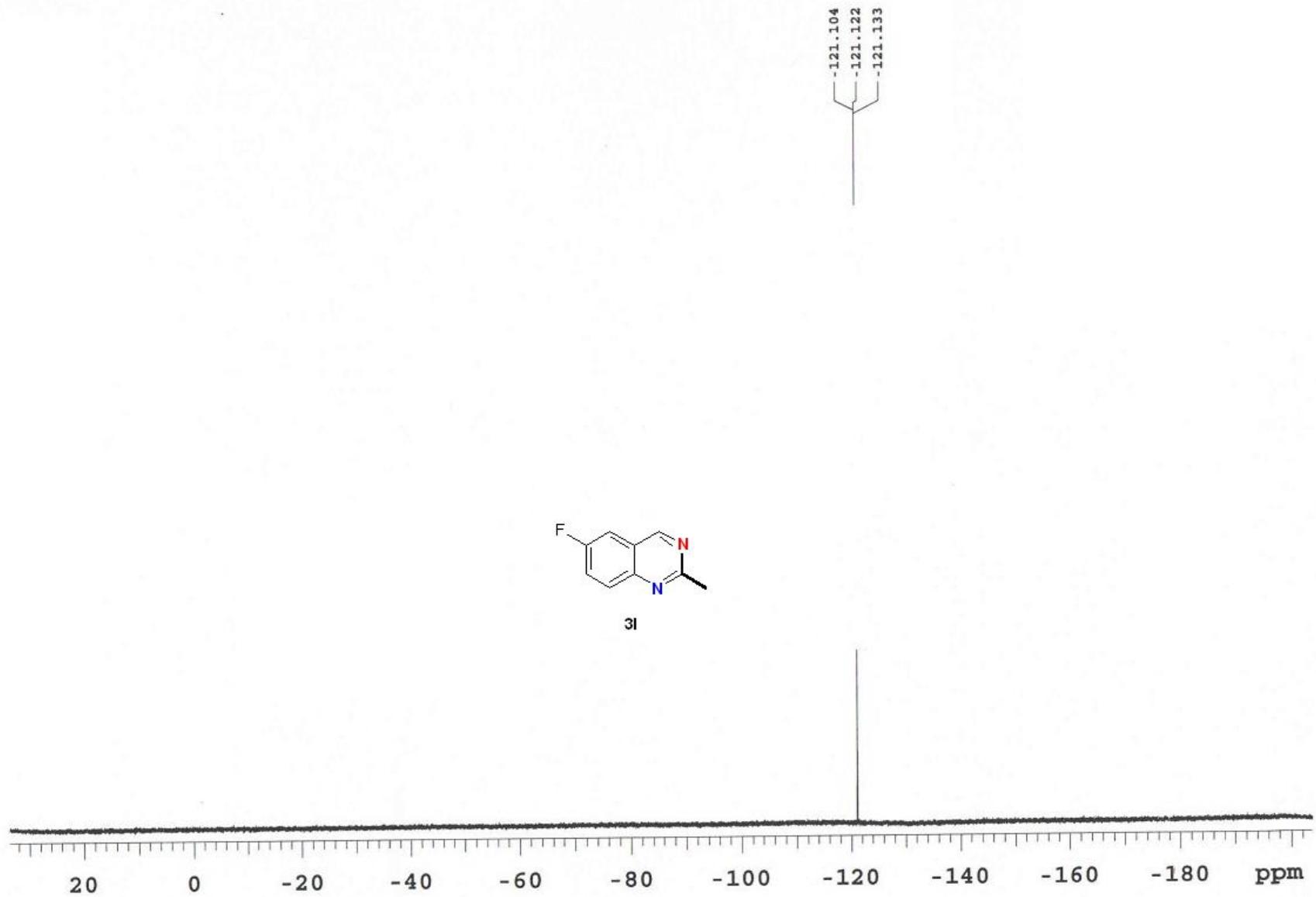




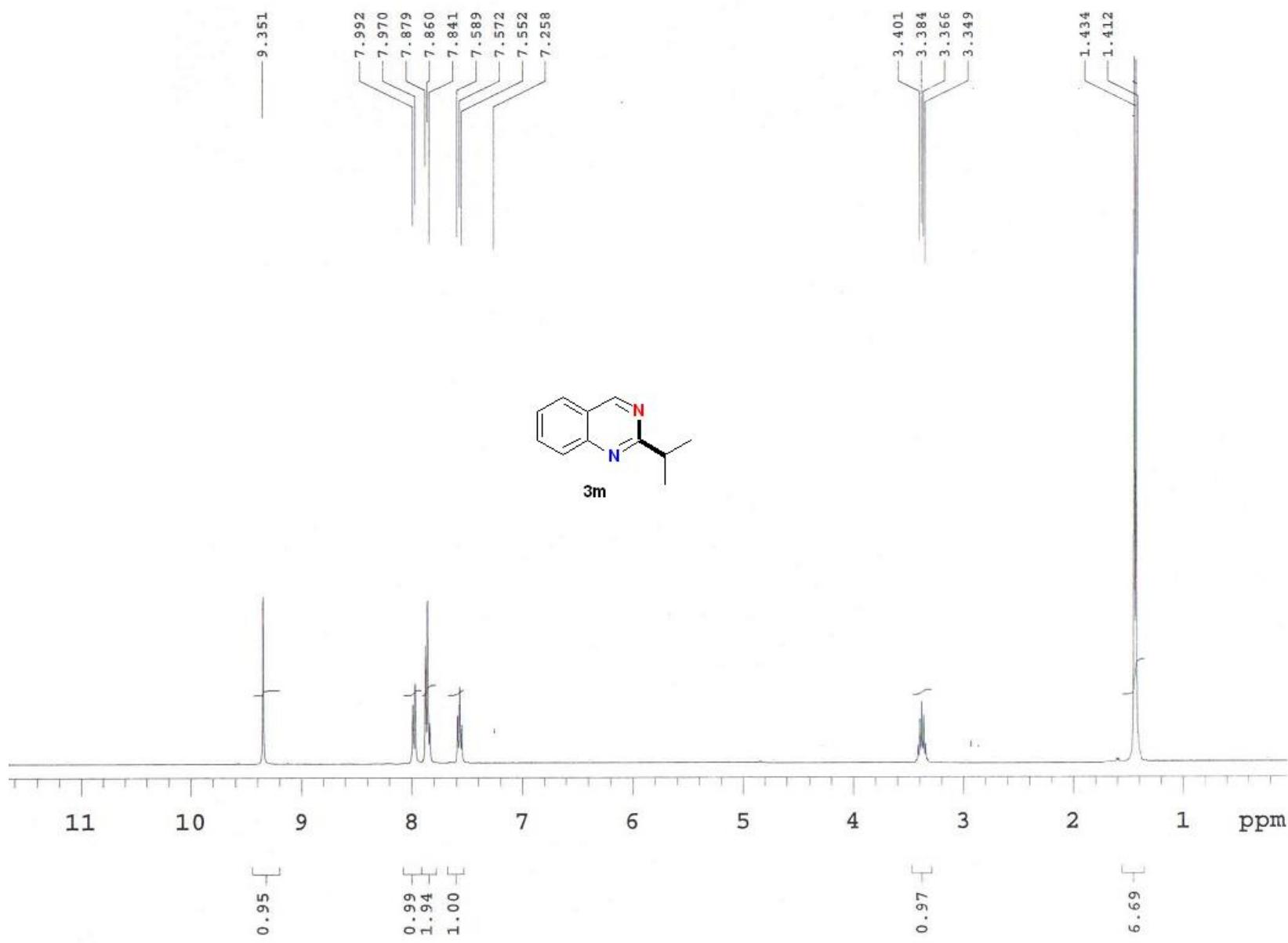
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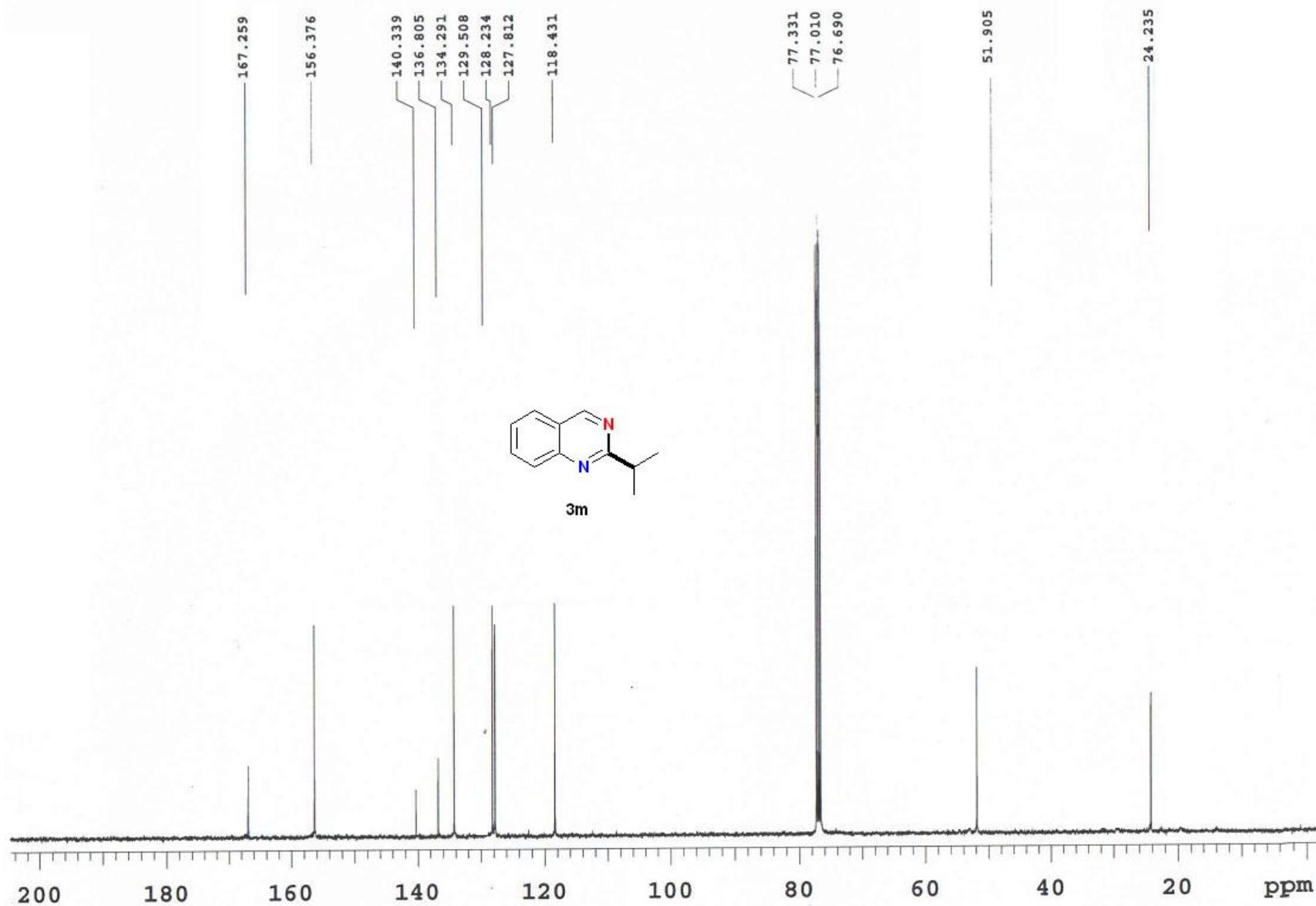
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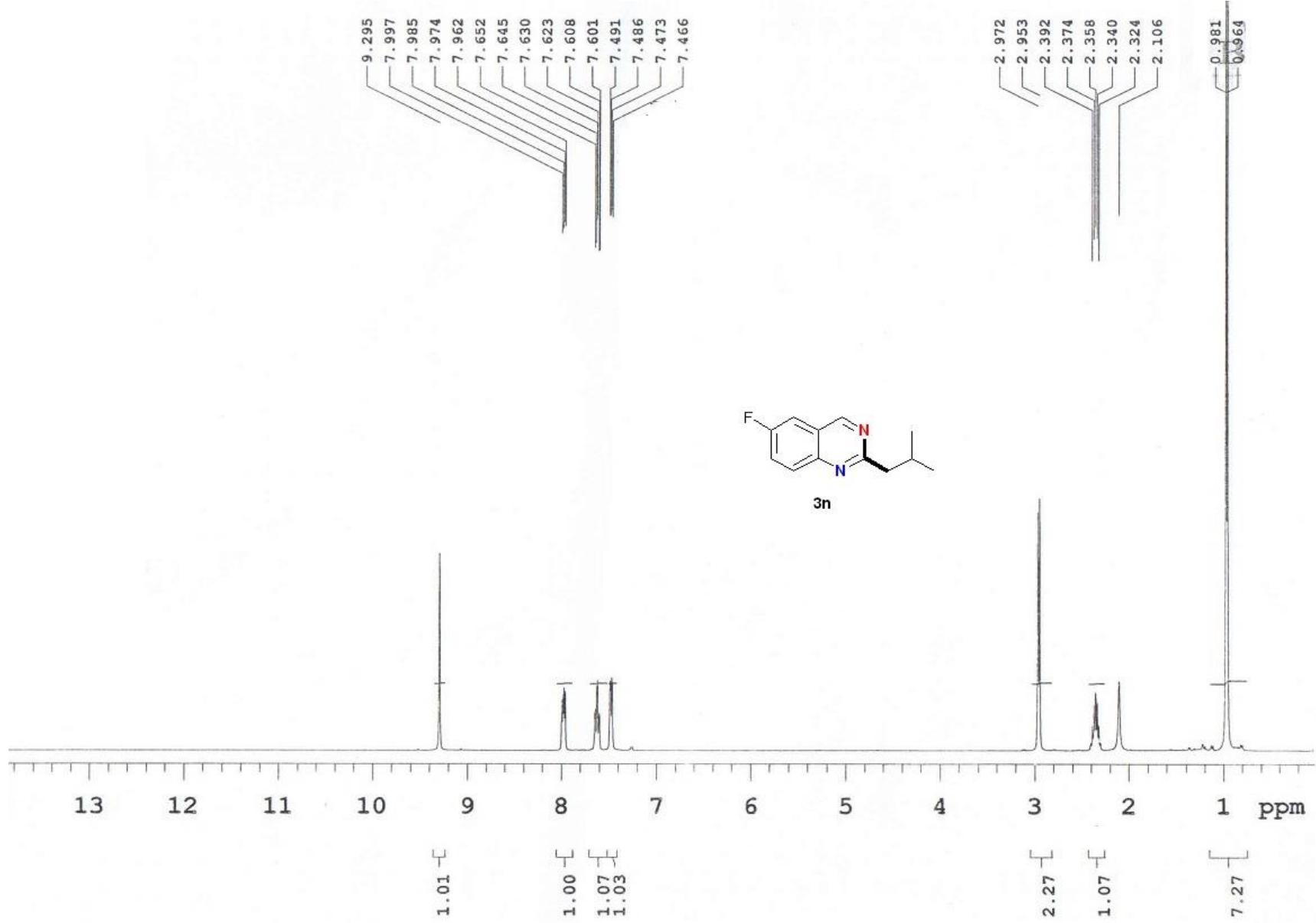


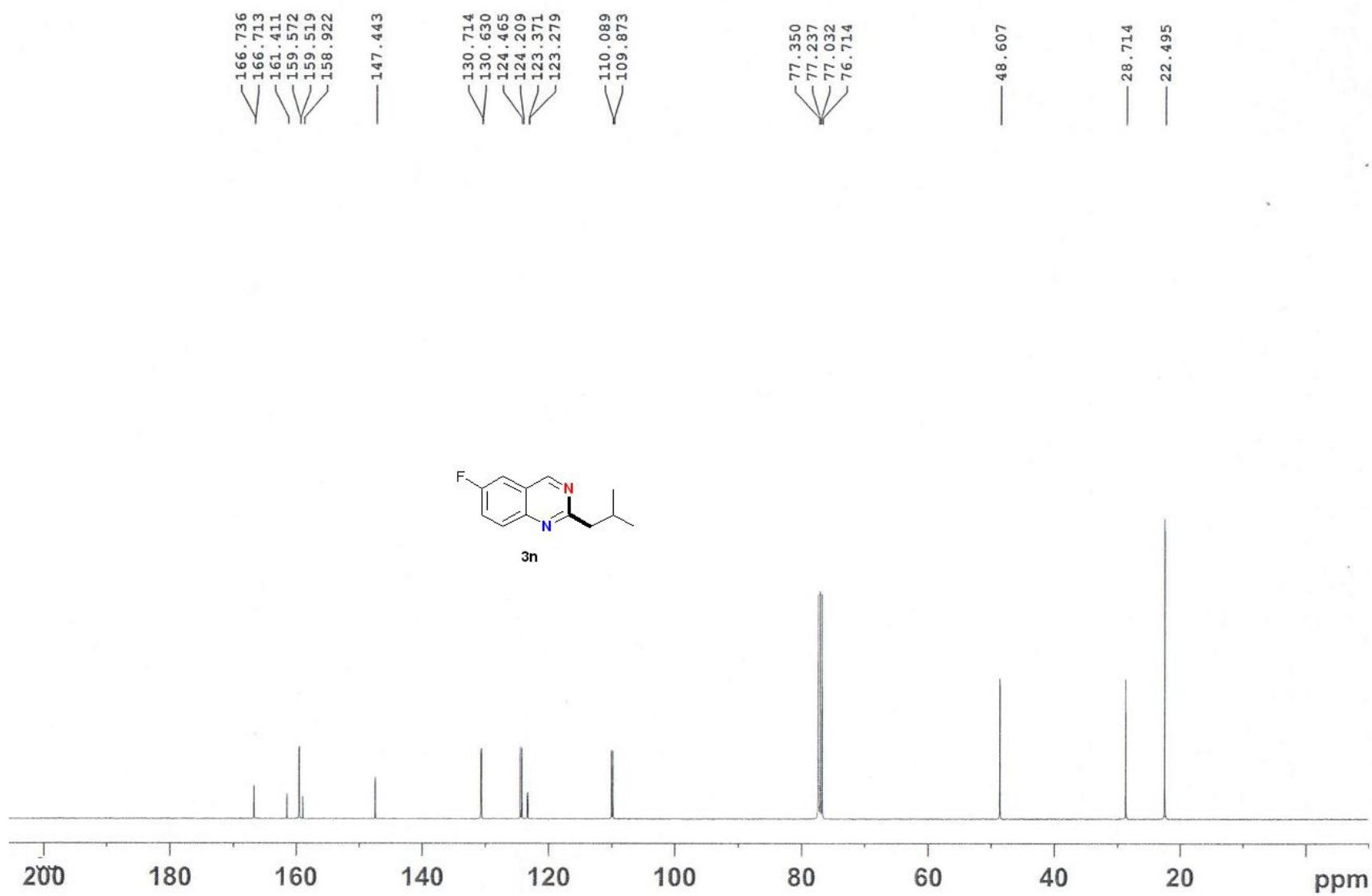
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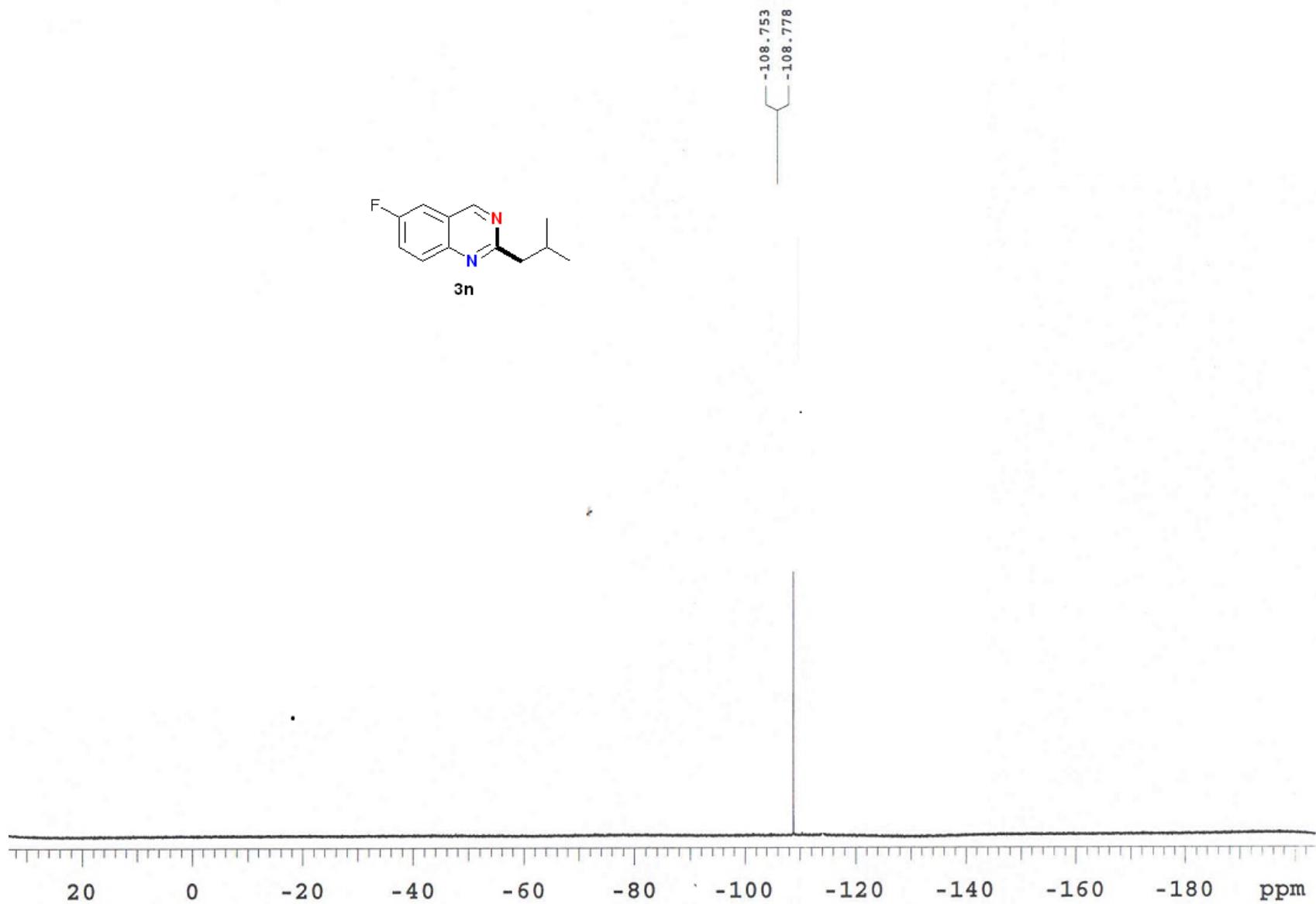
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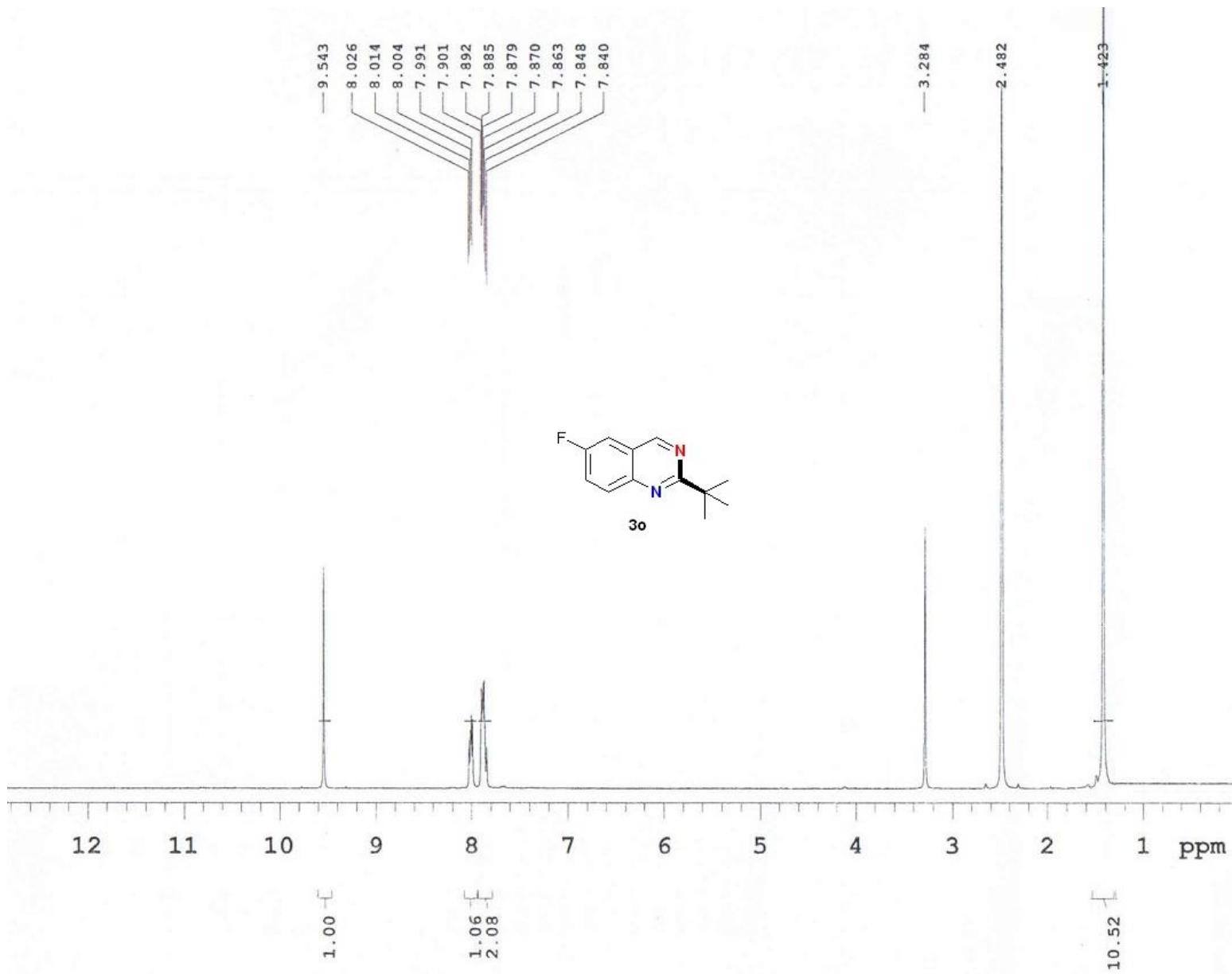


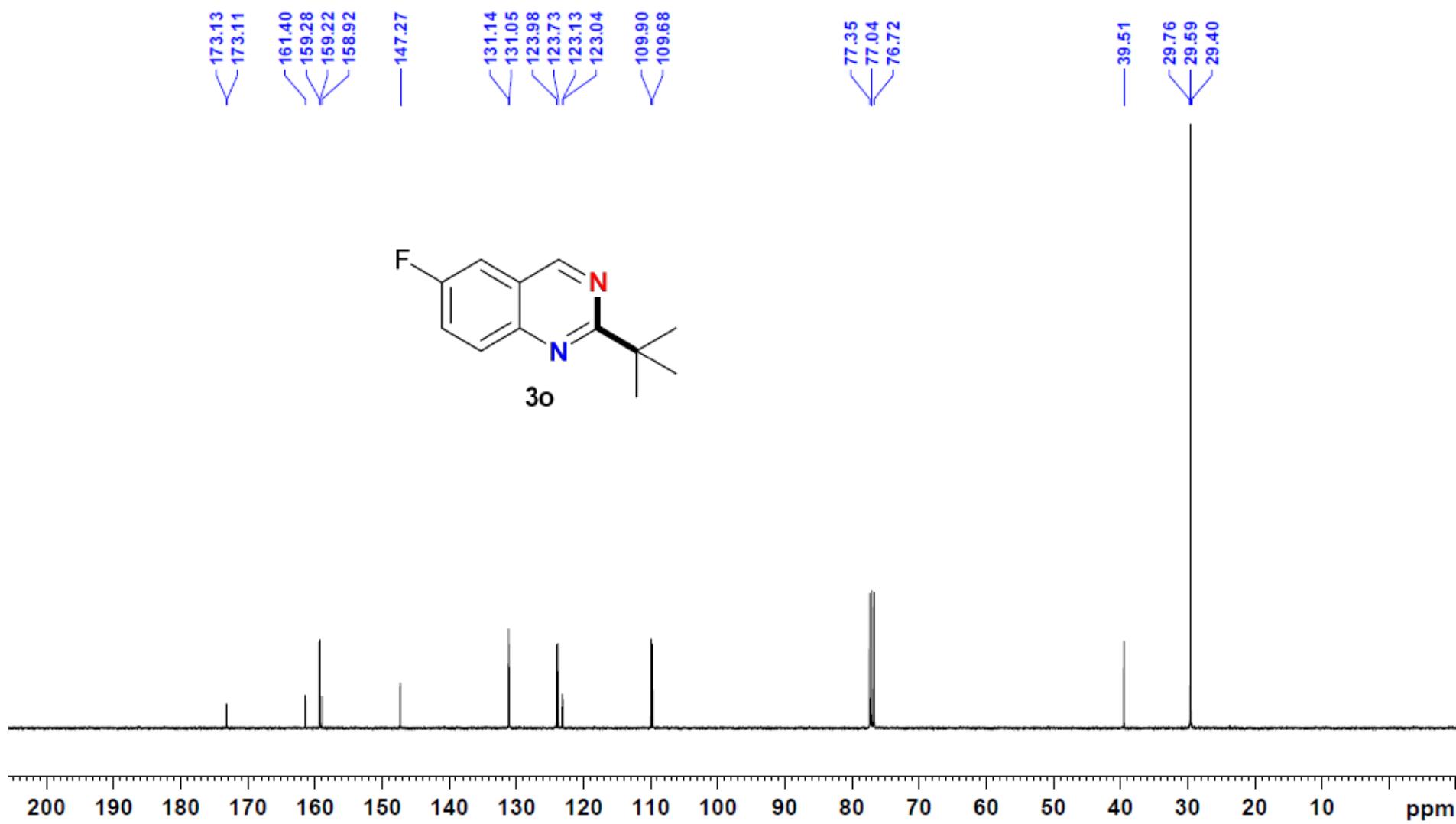


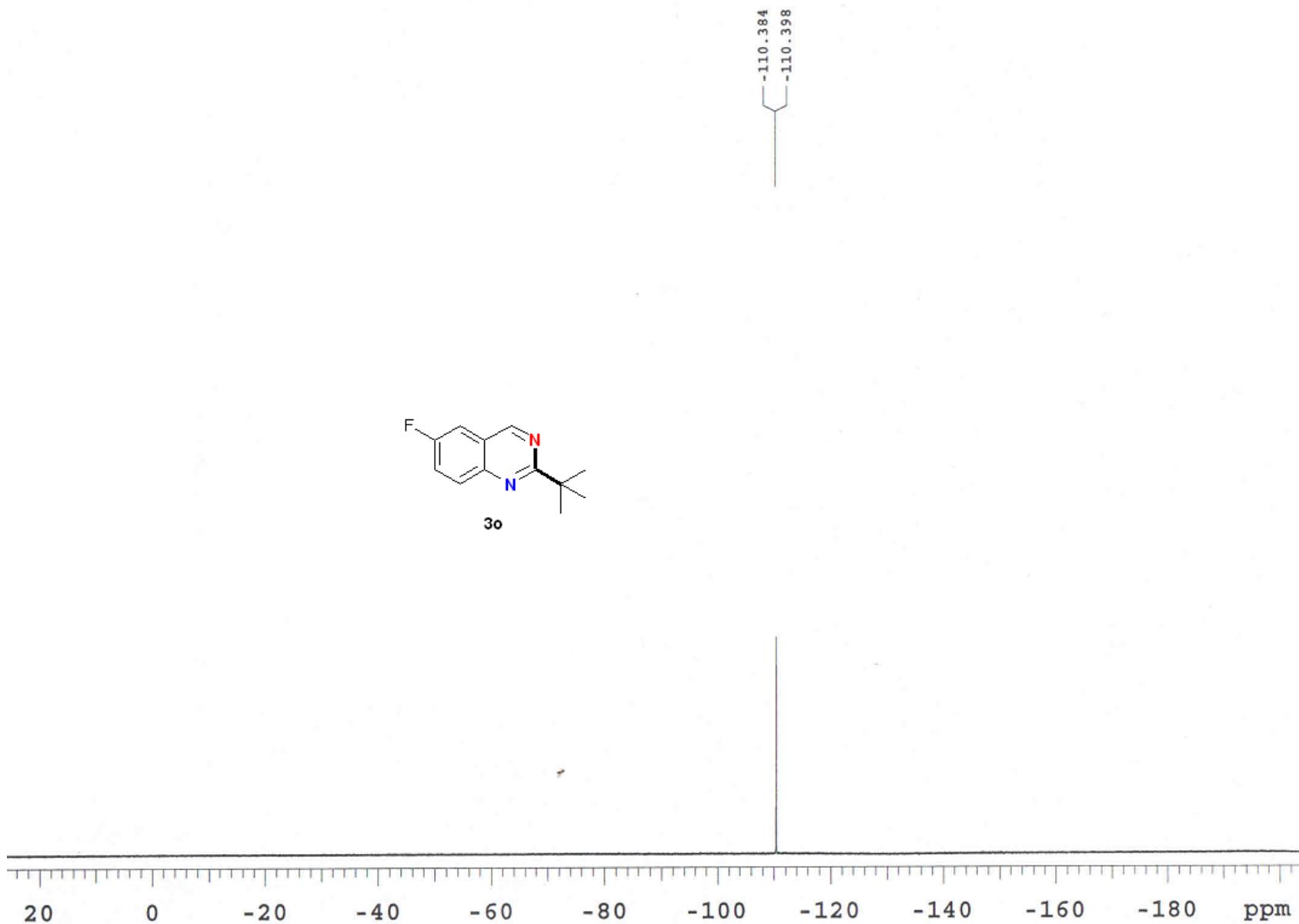
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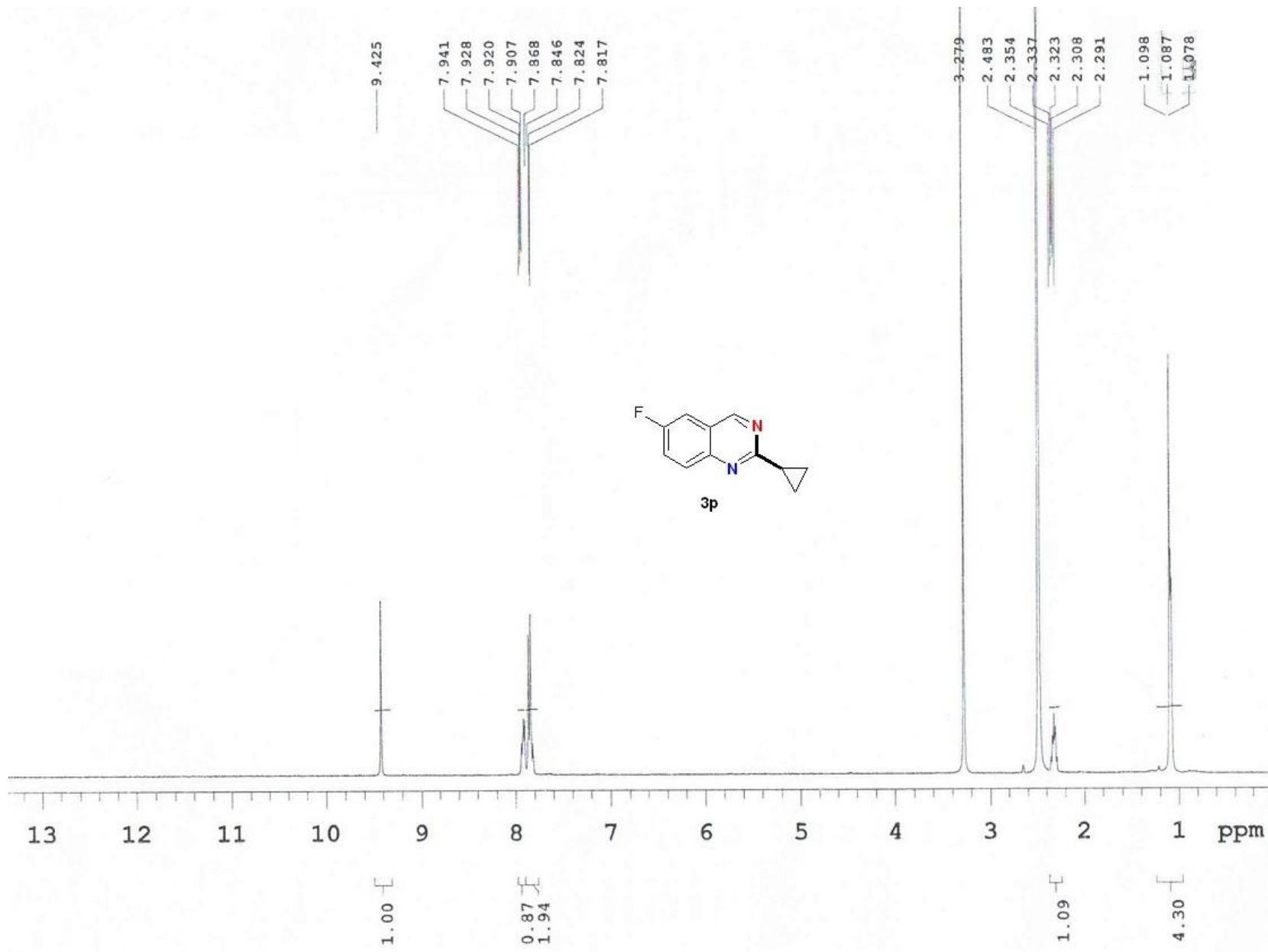
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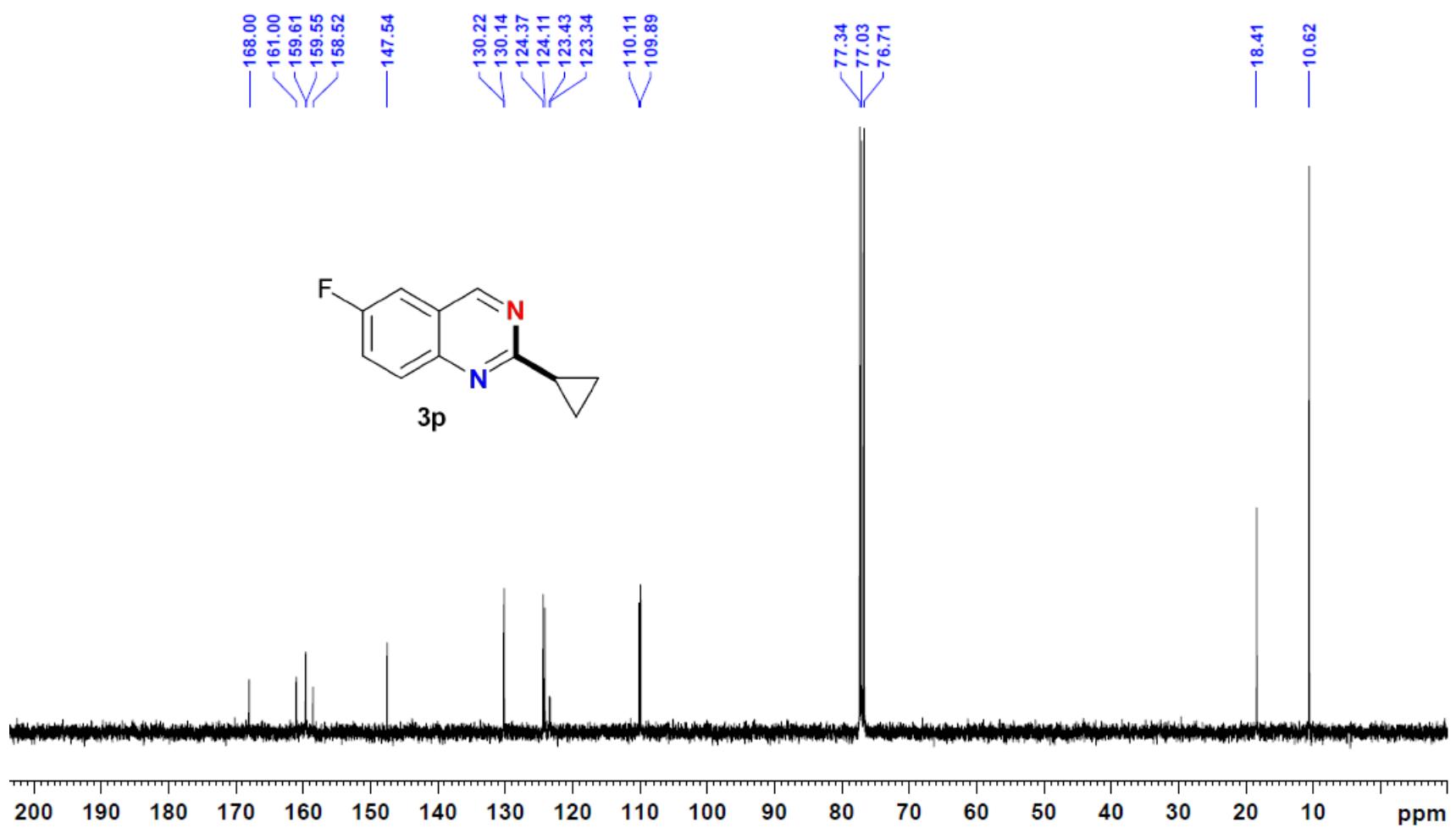


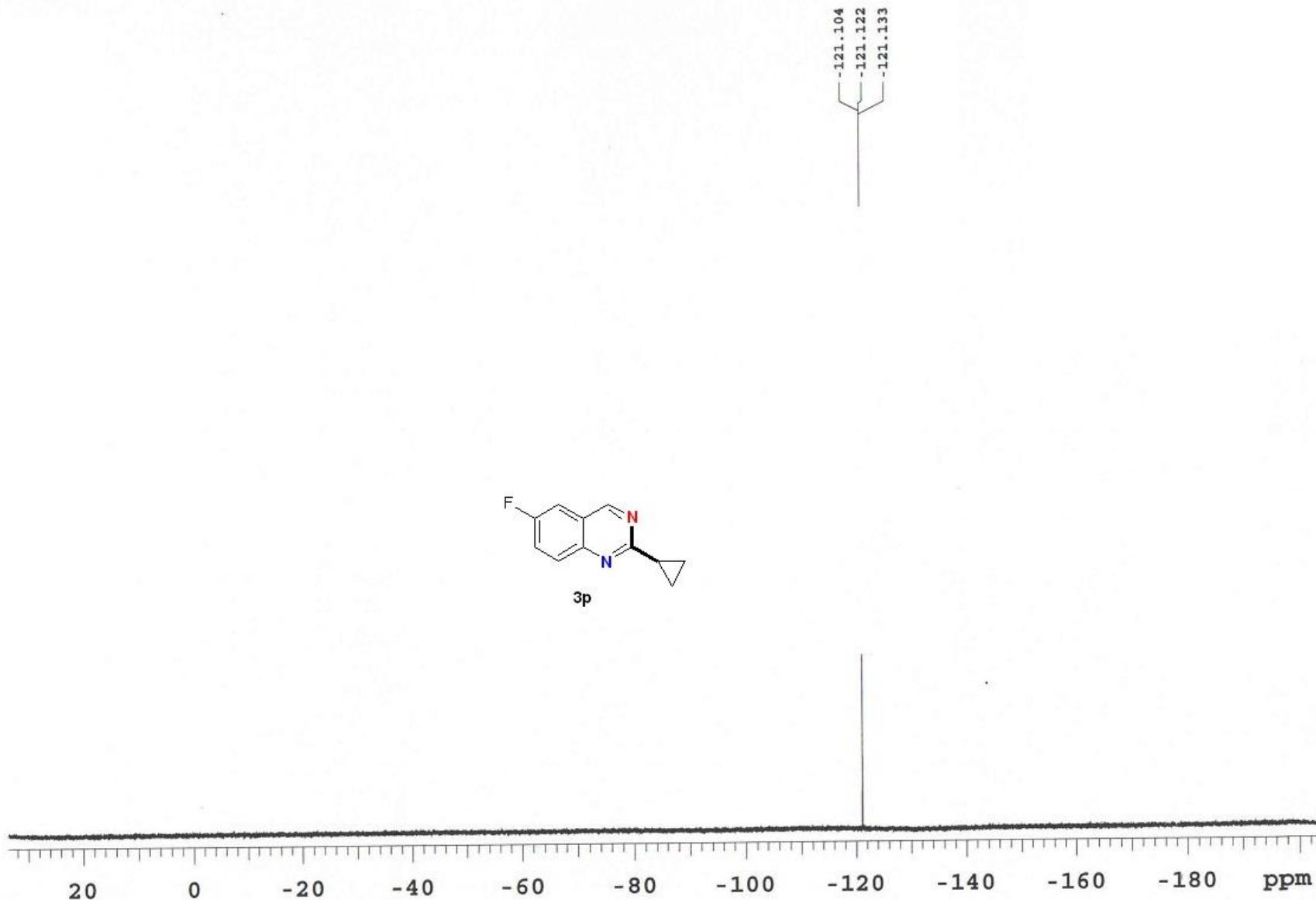


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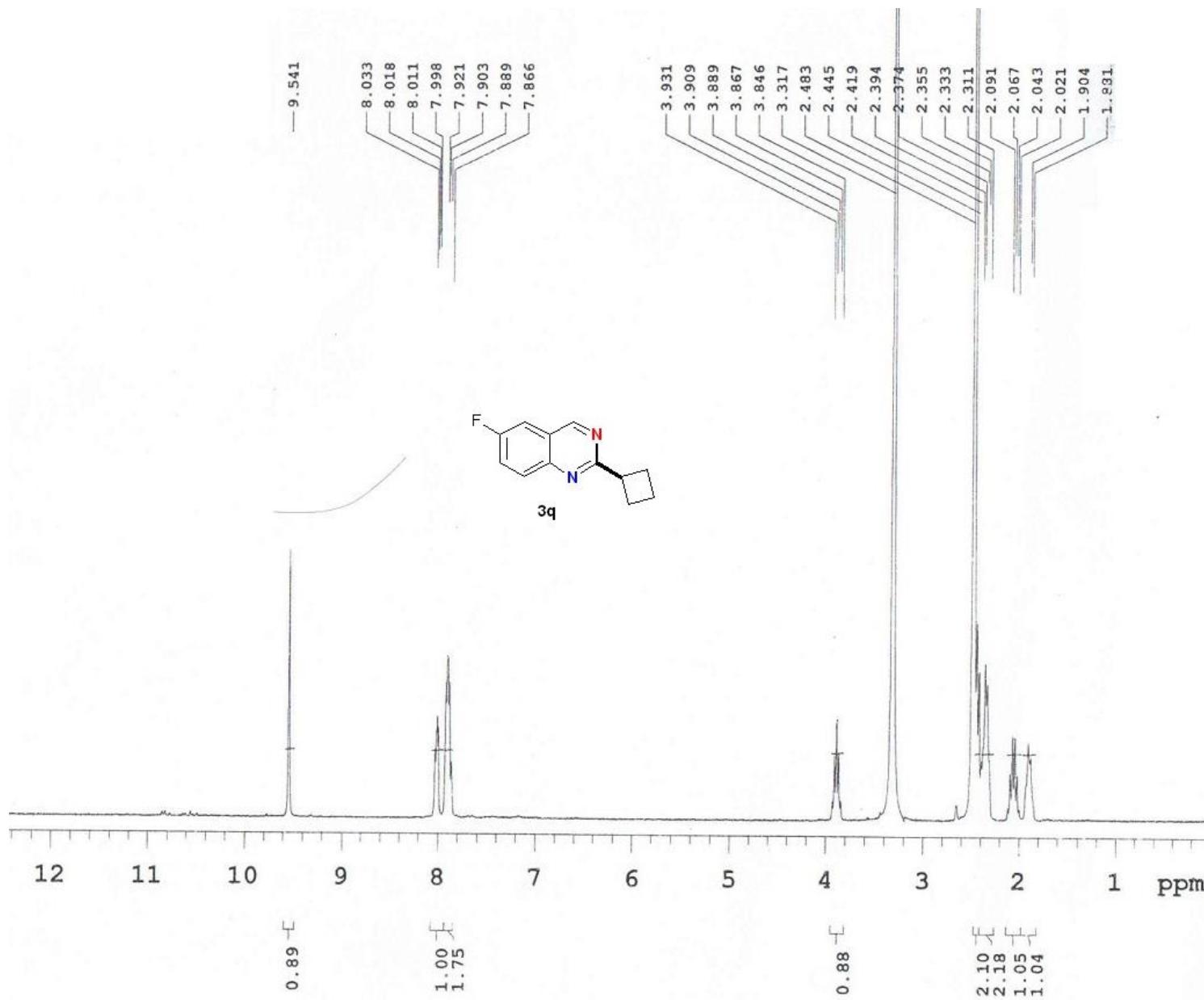


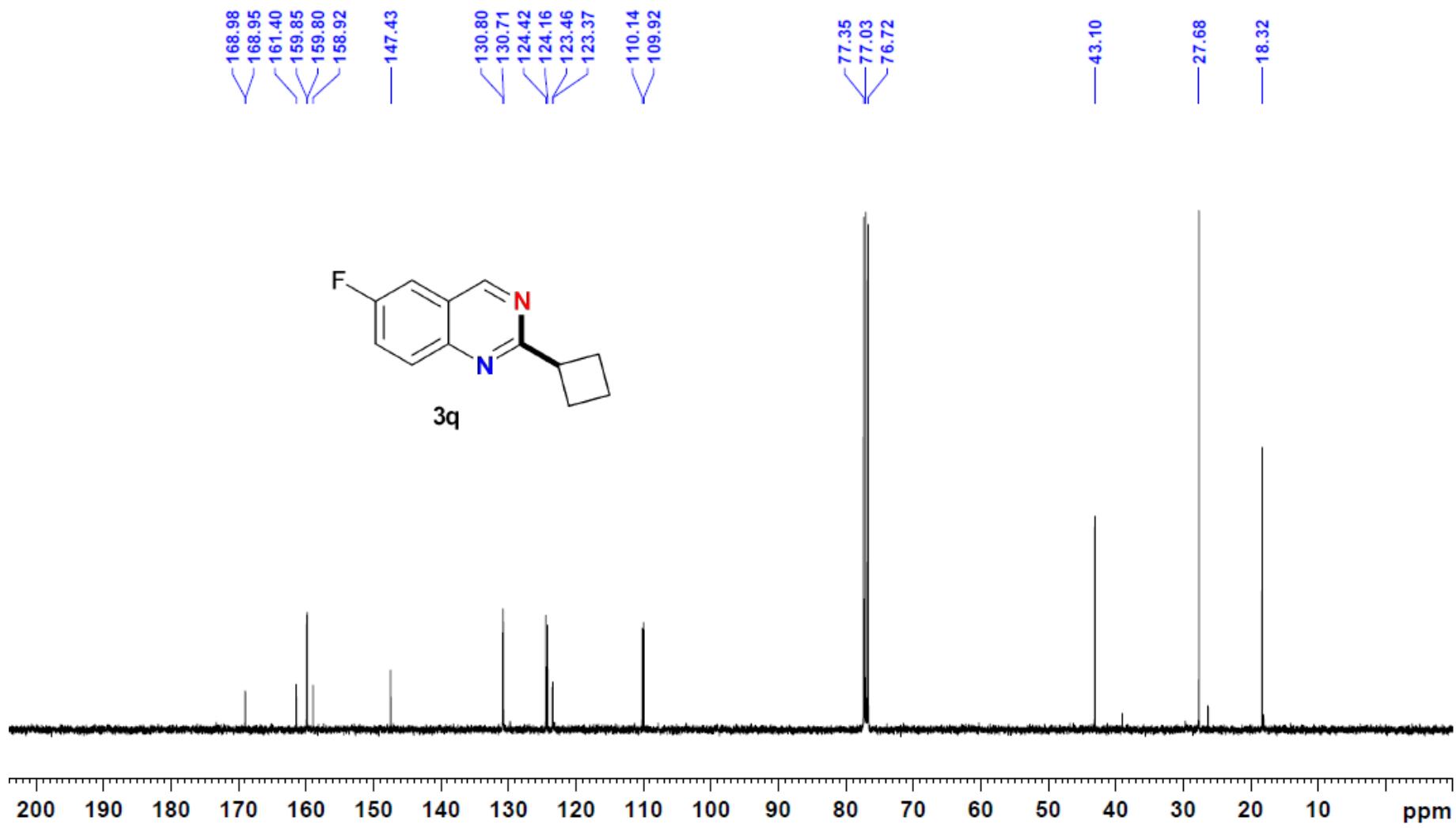
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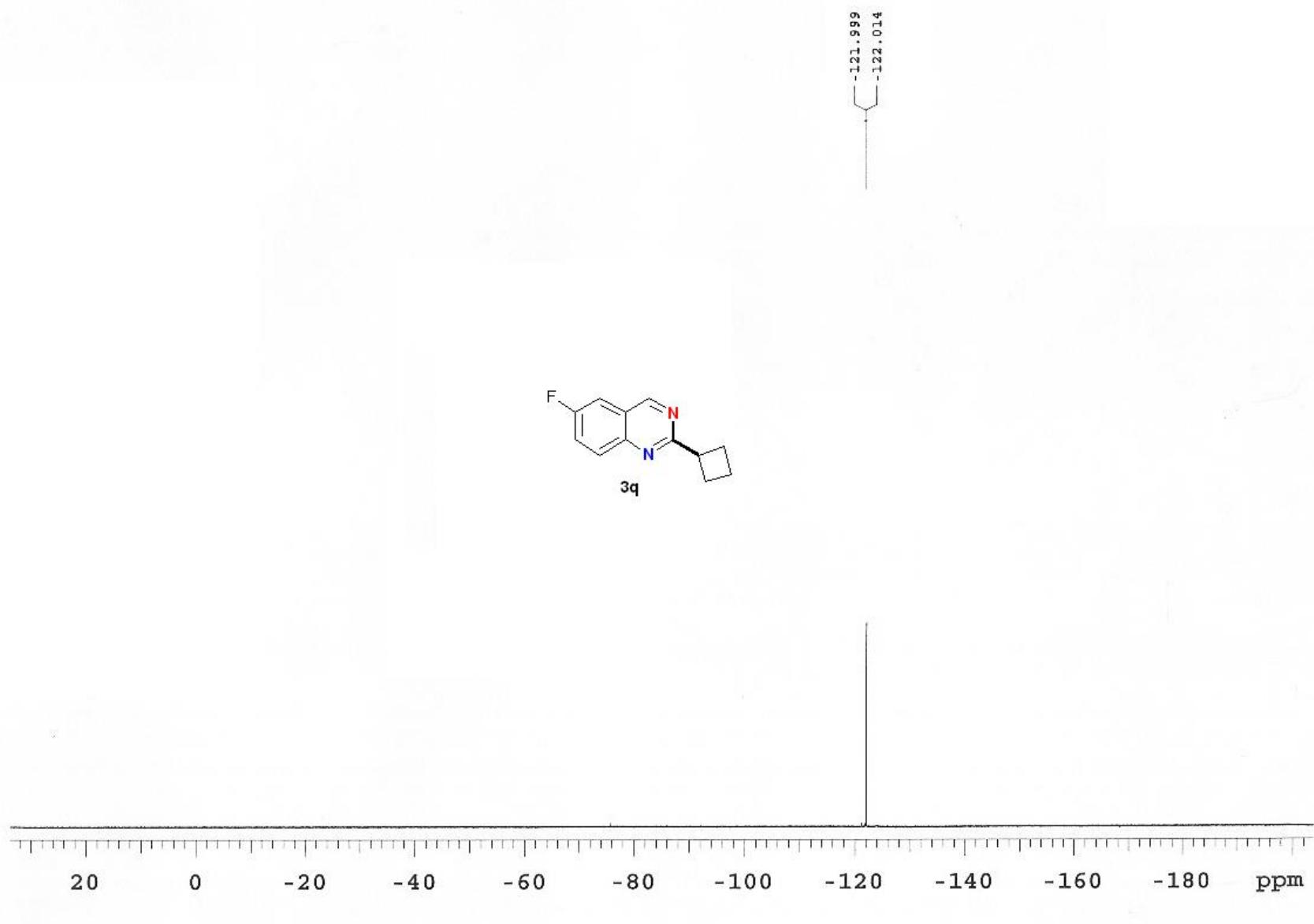


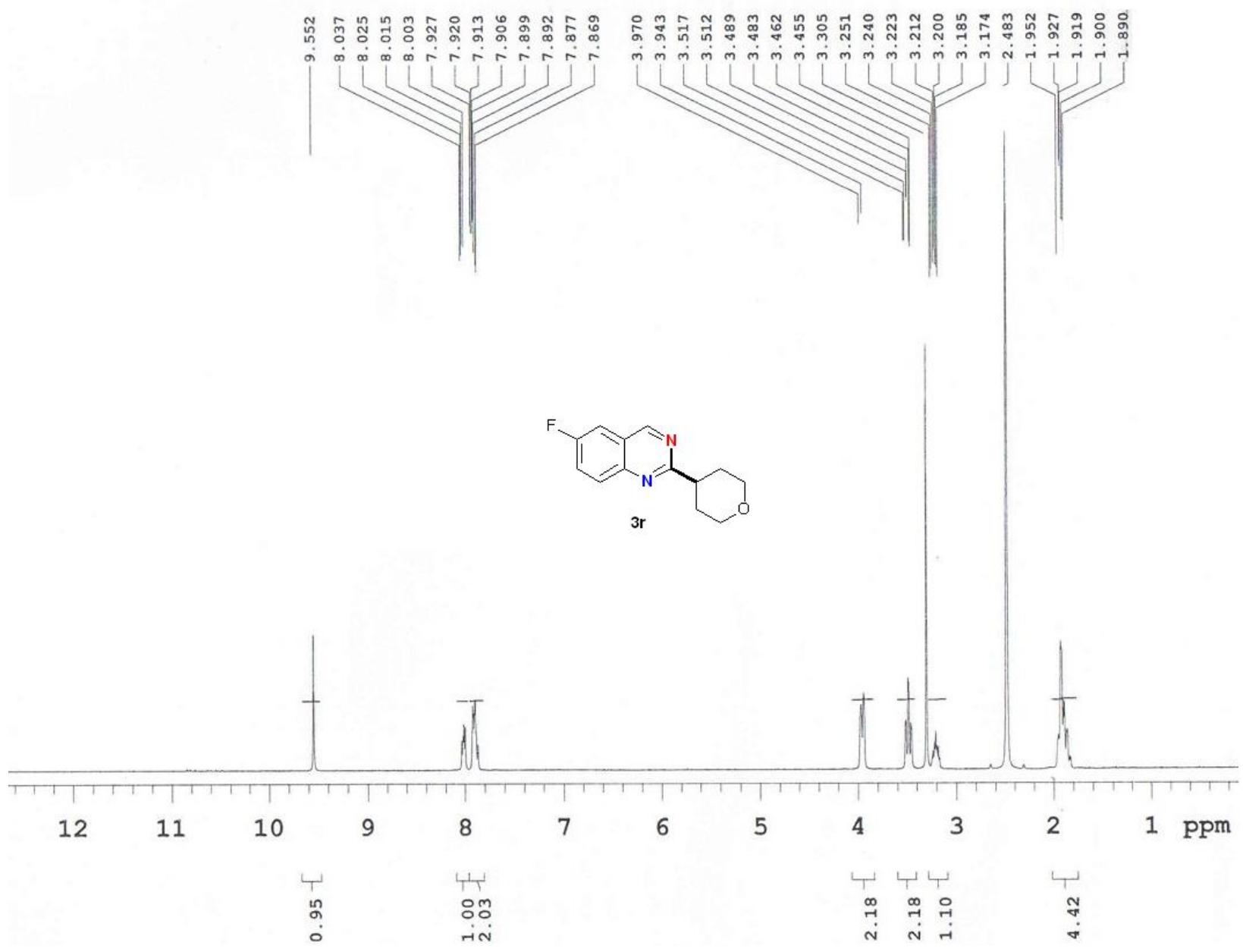


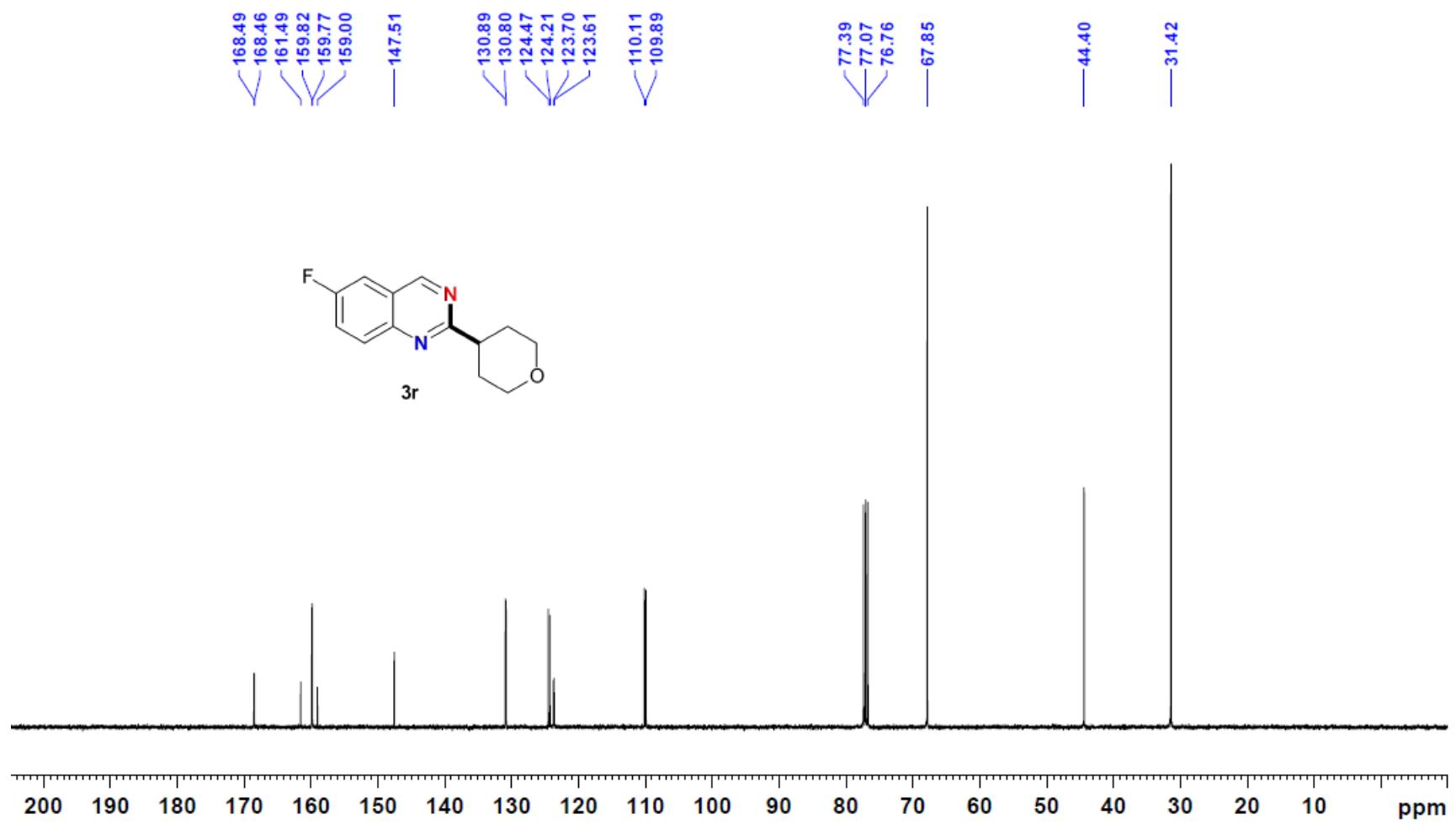
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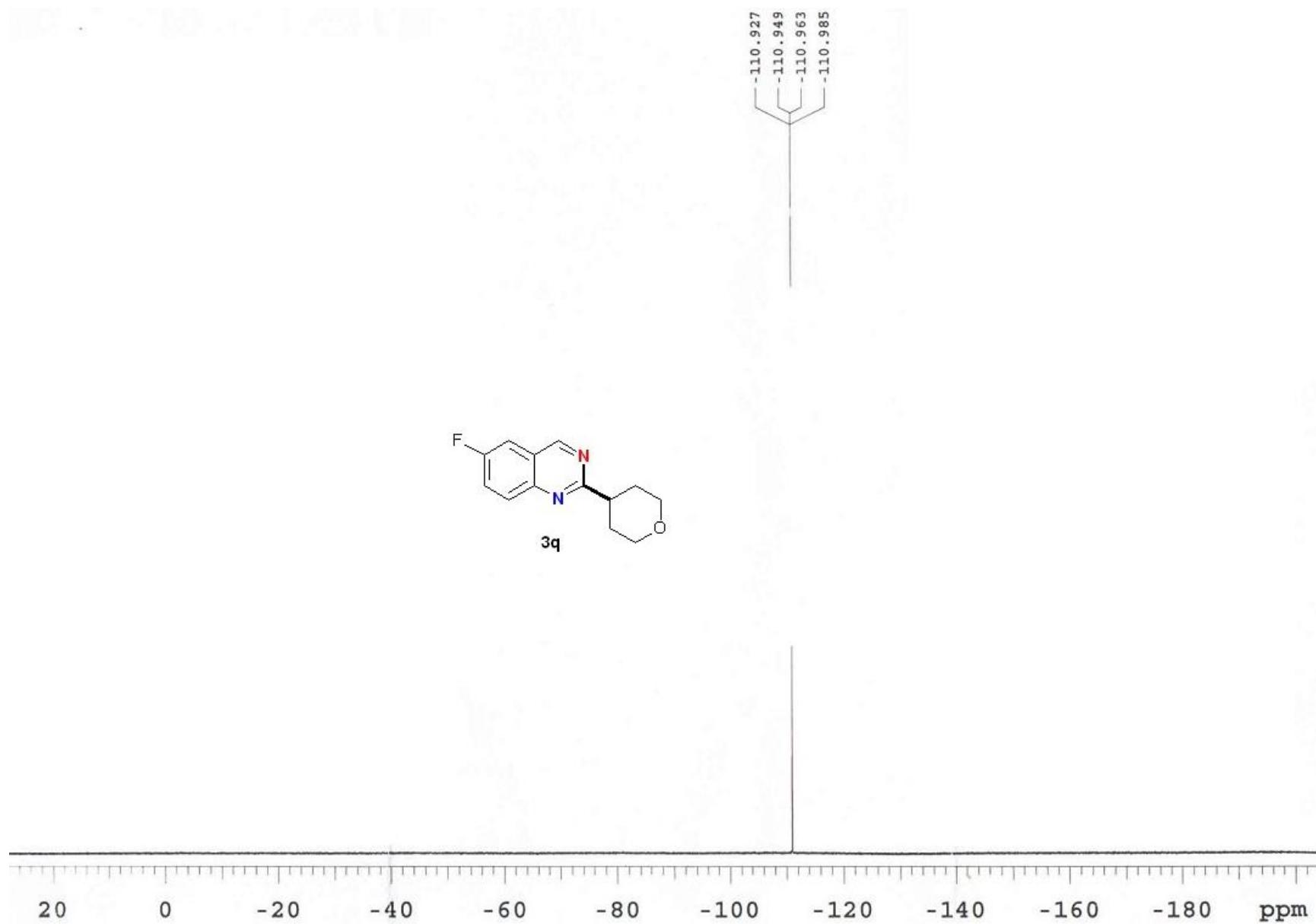


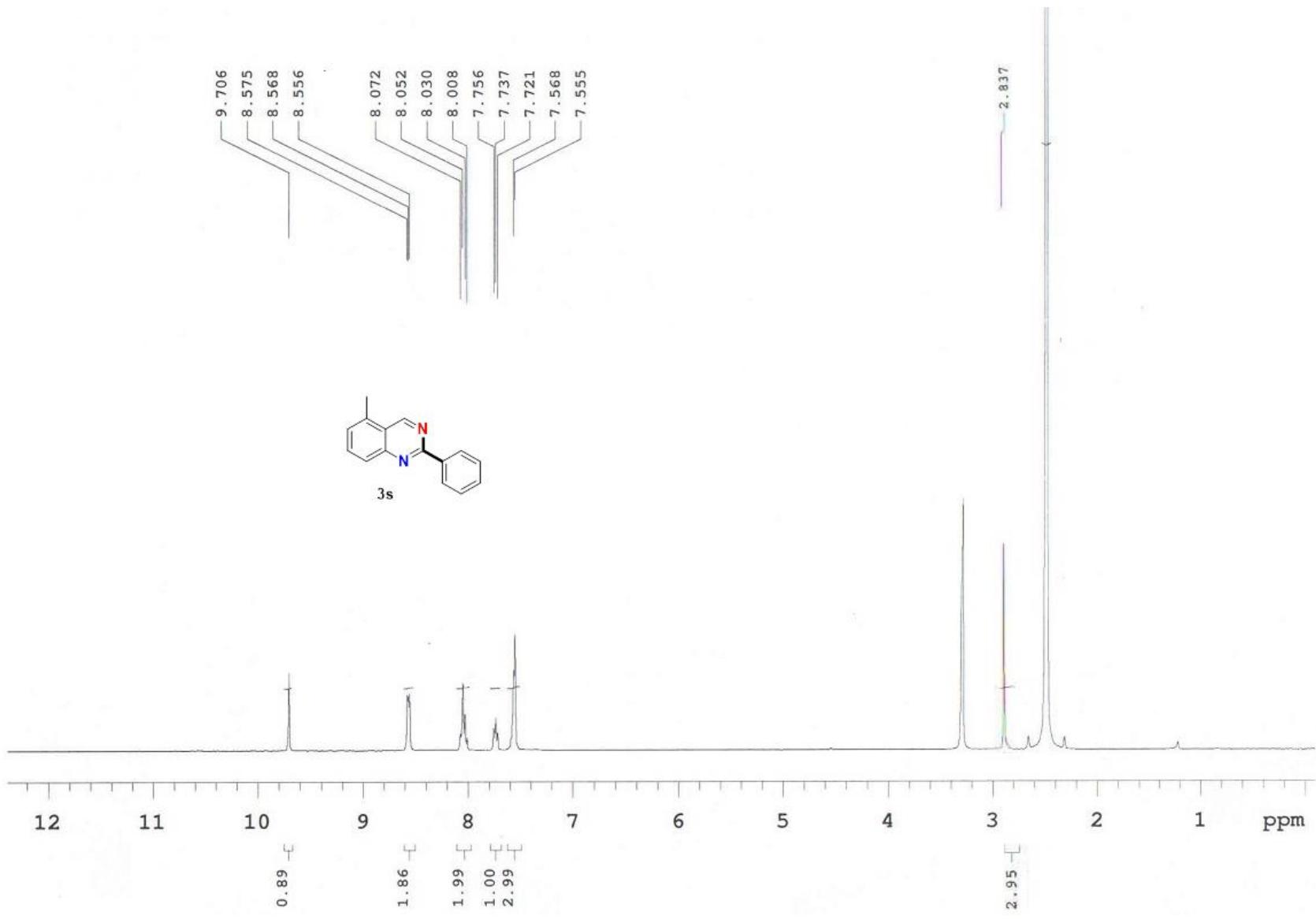


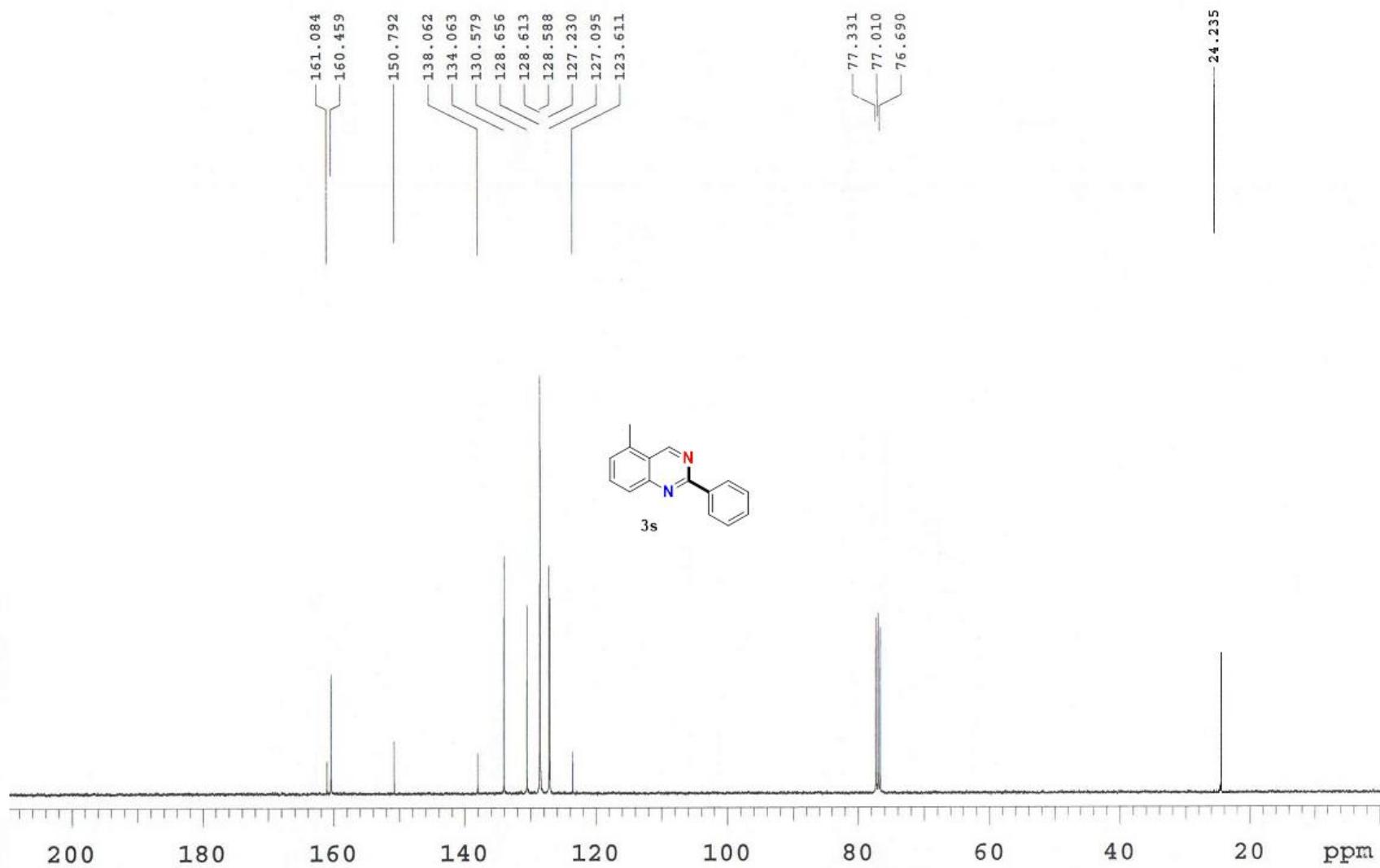




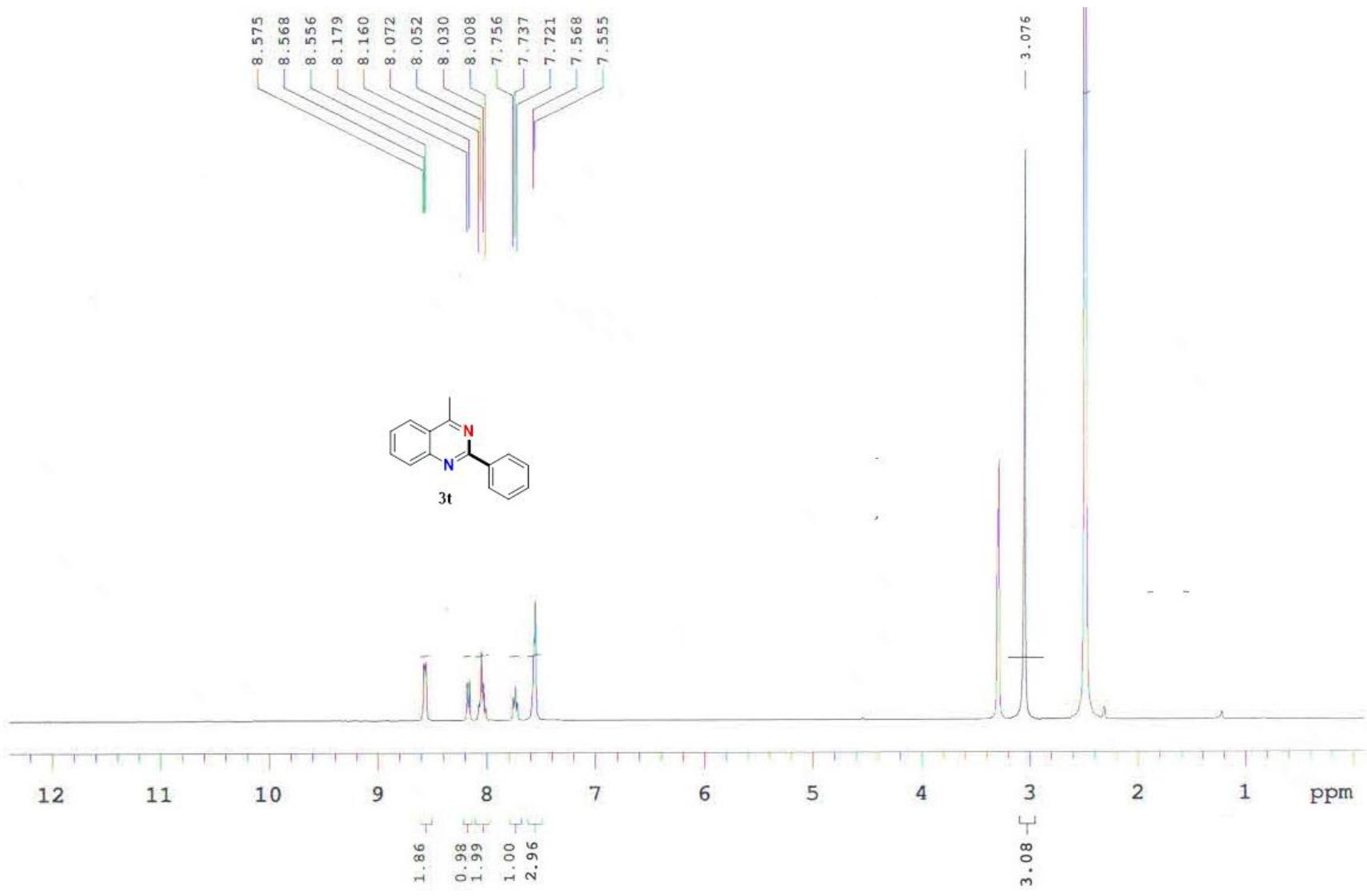


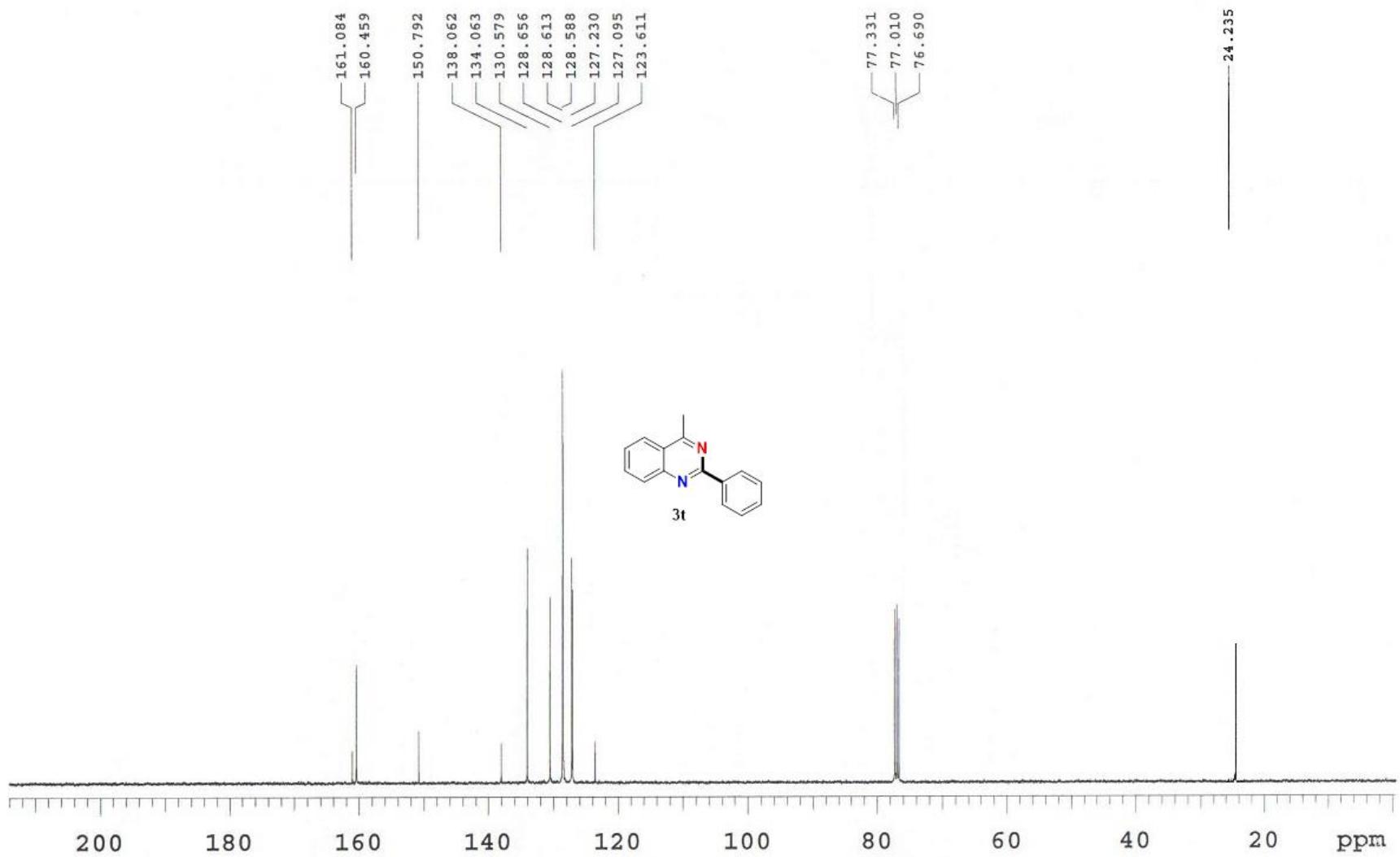




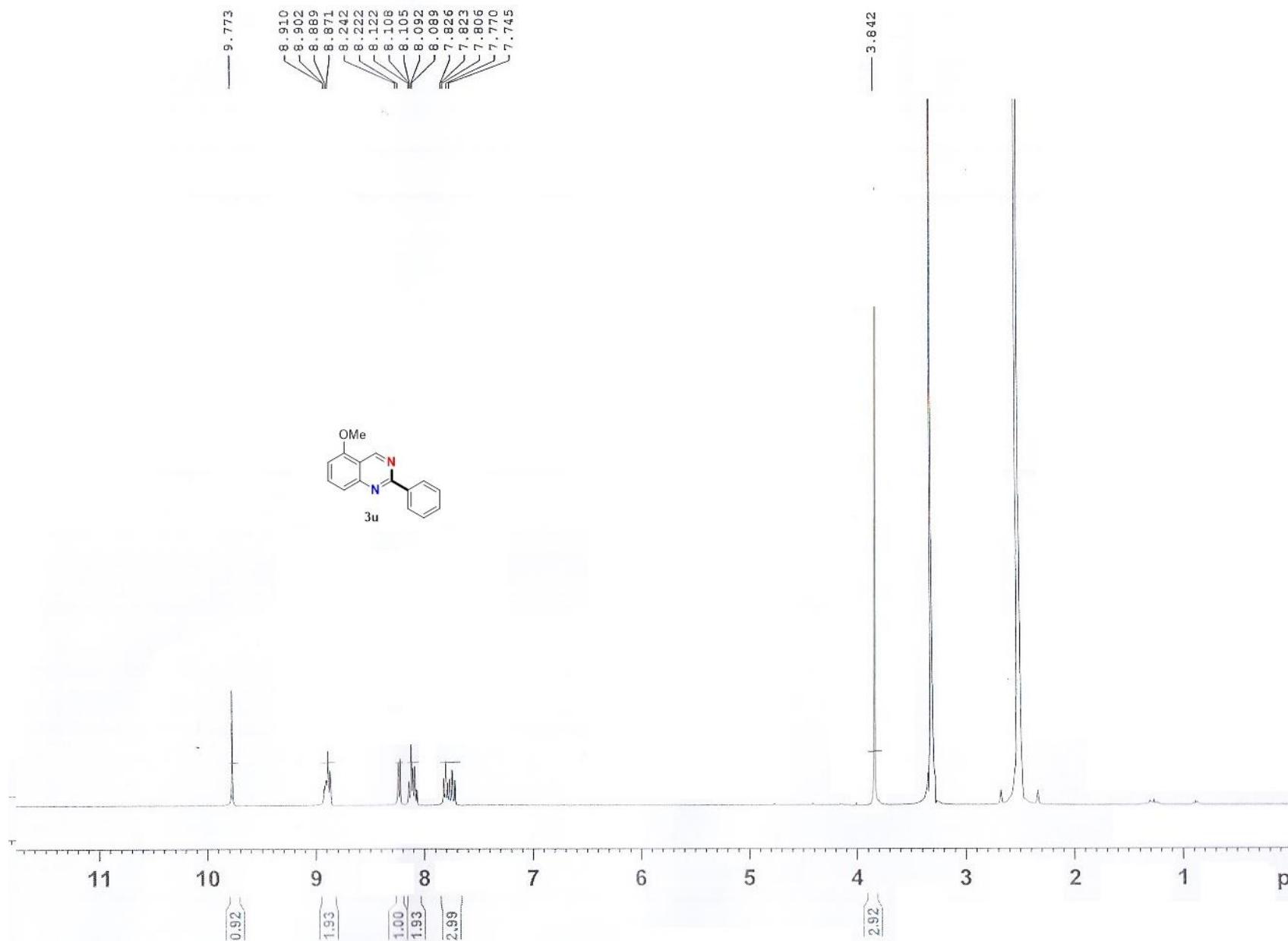


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